



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:59 AM EDT

PDB ID : 3M30 / pdb_00003m30
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

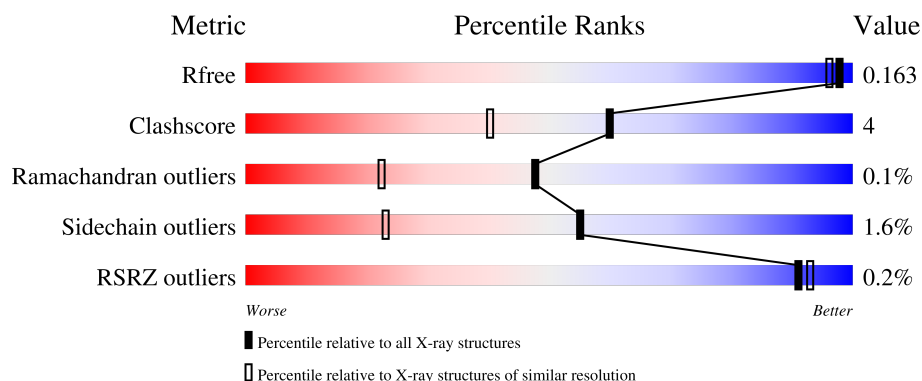
1 Overall quality at a glance

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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	85% 13% .
1	D	549	84% 15% .
2	B	442	83% 15% .
2	E	442	84% 15% .
3	C	248	% 82% 17% .

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Mol	Chain	Length	Quality of chain
3	F	248	% 78%18%...

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 [i](#)

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 (CCD ID: MG) (formula: Mg).

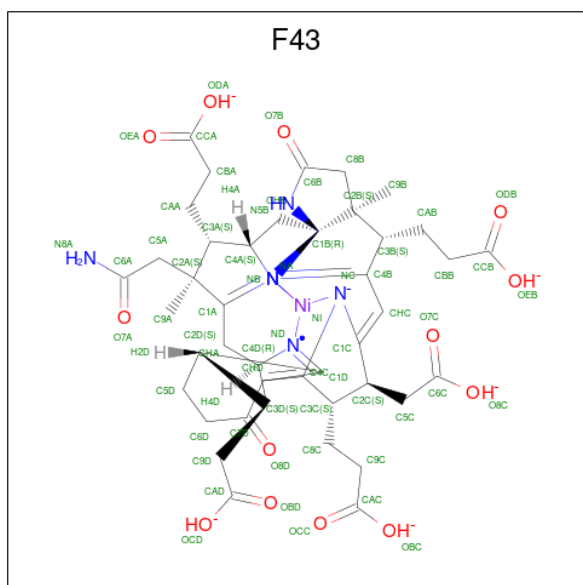
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	2	Total	Mg	0	0
			2	2		

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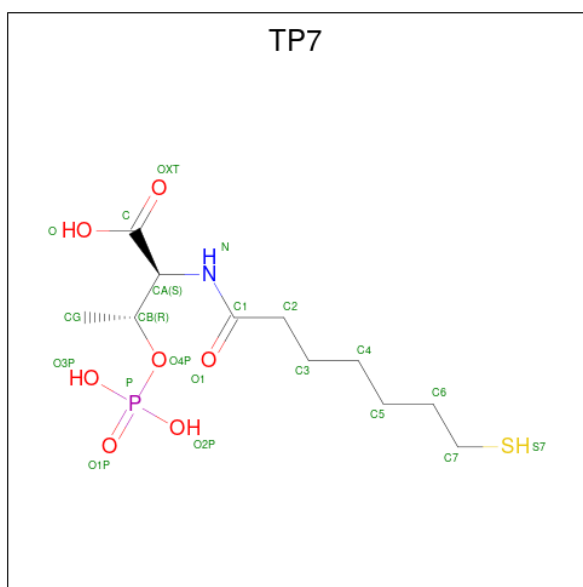
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

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



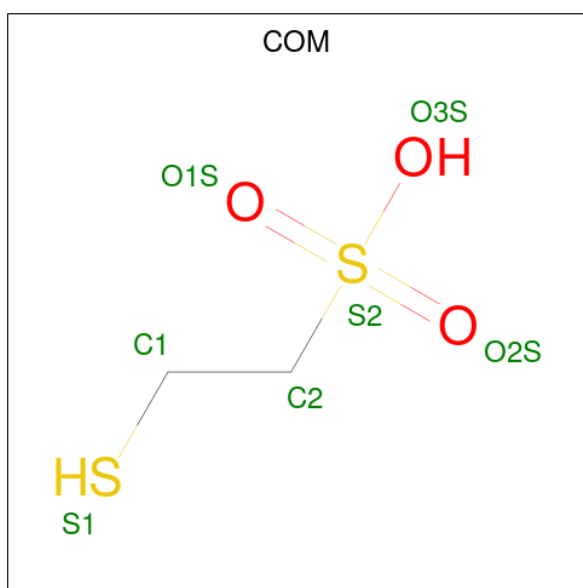
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

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



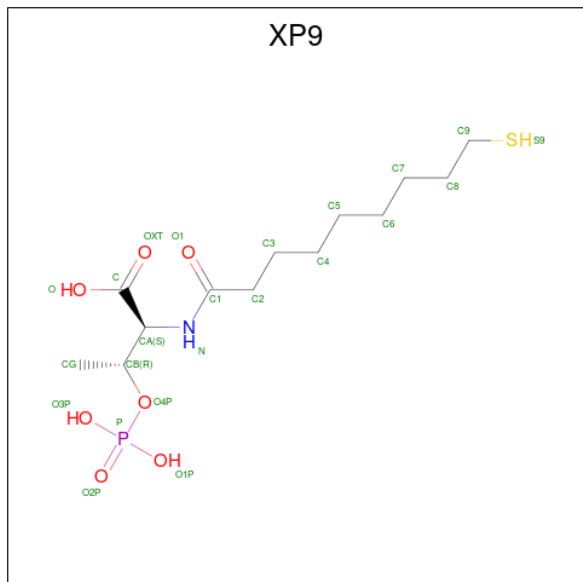
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

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



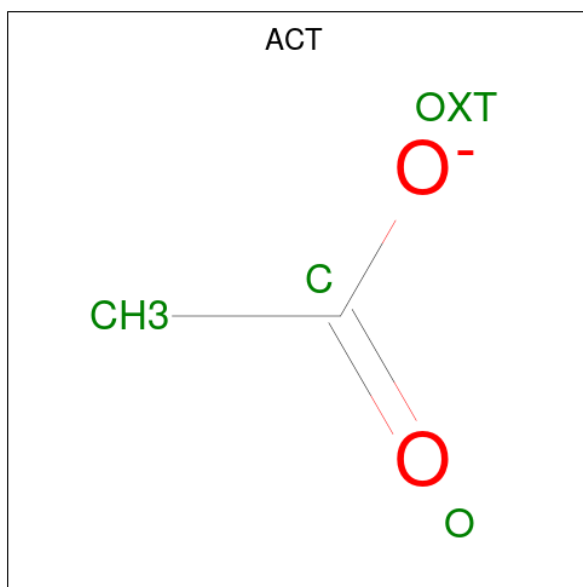
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

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



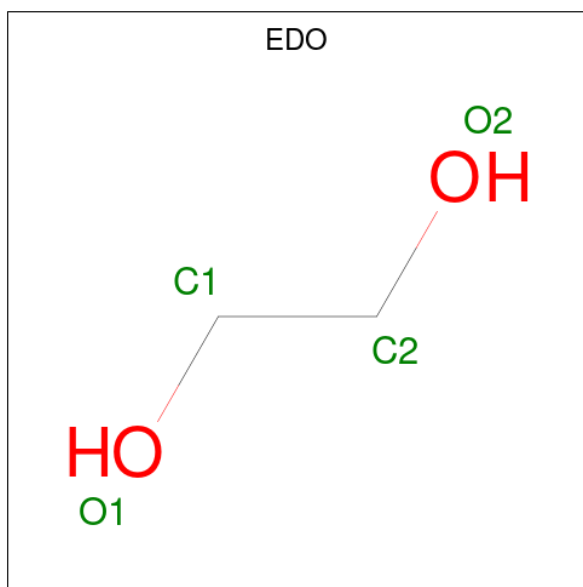
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			46	26	2	14	2	2		
8	D	1	Total	C	N	O	P	S	0	1
			46	26	2	14	2	2		

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



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

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

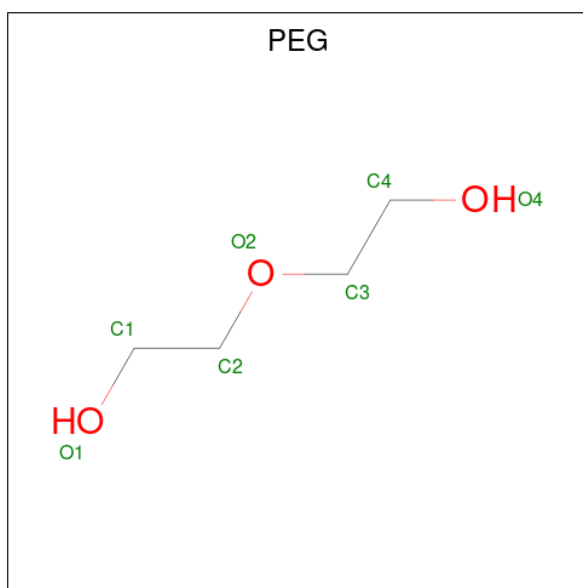


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

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

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

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



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

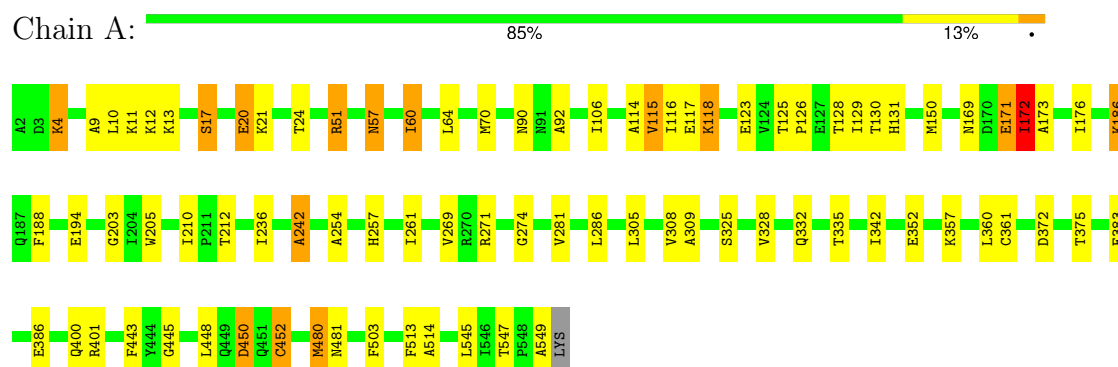
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	507	Total	O	0	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		

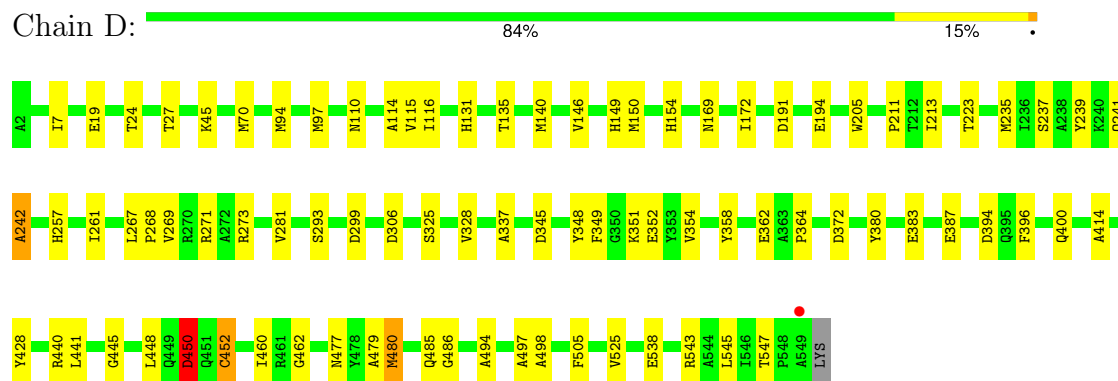
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

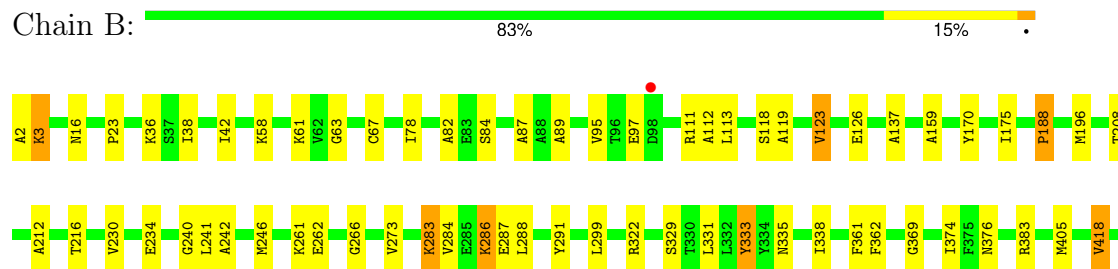
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



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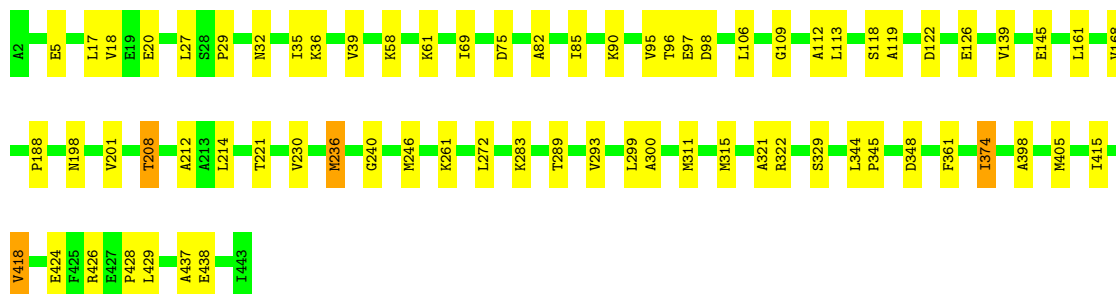
- Molecule 2: Methyl-coenzyme M reductase I subunit beta





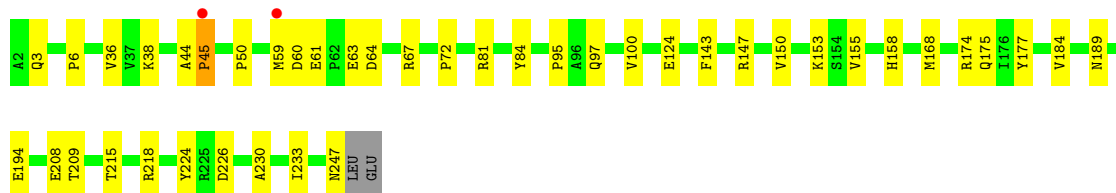
- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E: 84% 15%



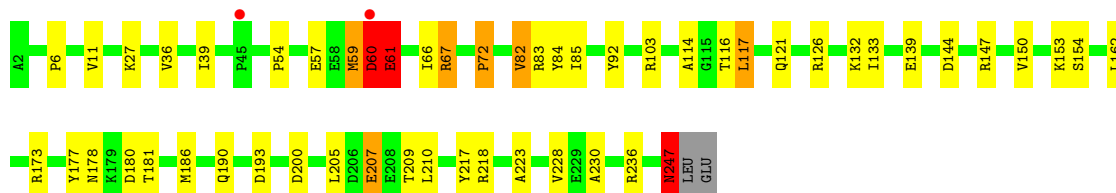
- Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C: 82% 17%



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

Chain F: 78% 18%



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 20.07 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.07-1.45) 97.6 (20.07-1.45)	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 (4.87%)	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 , 46.0	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: GL3, ZN, ACT, XP9, MHS, AGM, SMC, TP7, PEG, EDO, F43, MGN, MG, COM

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	1.76	43/4572 (0.9%)	1.48	22/6206 (0.4%)
1	D	1.80	46/4505 (1.0%)	1.49	19/6116 (0.3%)
2	B	1.74	34/3628 (0.9%)	1.42	12/4904 (0.2%)
2	E	1.75	32/3633 (0.9%)	1.42	5/4910 (0.1%)
3	C	1.86	22/2109 (1.0%)	1.51	5/2841 (0.2%)
3	F	1.83	26/2179 (1.2%)	1.53	10/2933 (0.3%)
All	All	1.78	203/20626 (1.0%)	1.47	73/27910 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	D	1	1
2	B	0	1
All	All	2	3

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	269	VAL	CA-CB	11.83	1.69	1.54
1	A	269	VAL	CA-CB	10.80	1.68	1.54
3	F	36	VAL	N-CA	9.55	1.57	1.46
2	B	286	LYS	N-CA	8.65	1.56	1.45
3	F	210	LEU	N-CA	8.27	1.56	1.46
1	A	547	THR	N-CA	8.14	1.52	1.45
1	A	60	ILE	CA-CB	8.09	1.64	1.54
1	D	110	ASN	N-CA	7.79	1.55	1.46
2	B	16	ASN	N-CA	7.67	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	THR	C-O	7.50	1.32	1.24
1	A	172	ILE	CA-CB	7.26	1.63	1.54
2	B	87	ALA	CA-CB	7.11	1.64	1.53
2	B	240	GLY	N-CA	6.96	1.54	1.45
2	B	89	ALA	N-CA	6.95	1.54	1.46
3	C	36	VAL	CA-CB	-6.95	1.45	1.54
2	B	38	ILE	CA-CB	6.91	1.63	1.54
1	D	494	ALA	N-CA	6.88	1.53	1.46
3	F	6	PRO	C-N	6.83	1.38	1.33
3	C	209	THR	CA-C	6.73	1.61	1.52
1	D	486	GLY	CA-C	6.71	1.60	1.51
1	A	60	ILE	C-O	-6.69	1.16	1.24
1	D	140	MET	N-CA	6.69	1.53	1.46
3	C	168	MET	N-CA	6.61	1.54	1.46
3	F	247	ASN	CA-CB	6.57	1.66	1.53
1	D	543	ARG	N-CA	6.56	1.53	1.46
3	F	82	VAL	N-CA	6.53	1.54	1.46
2	E	161	LEU	N-CA	6.53	1.54	1.45
3	F	139	GLU	N-CA	6.53	1.54	1.46
1	A	11	LYS	N-CA	6.49	1.54	1.46
1	D	27	THR	CA-CB	6.48	1.63	1.53
1	D	364	PRO	CA-C	6.47	1.60	1.52
1	A	64	LEU	C-O	6.46	1.31	1.23
2	E	106	LEU	CA-C	-6.40	1.44	1.52
2	B	291	TYR	N-CA	6.38	1.54	1.46
2	B	266	GLY	C-O	6.38	1.31	1.23
3	C	6	PRO	N-CA	6.38	1.54	1.46
2	B	170	TYR	CA-CB	6.36	1.60	1.52
2	E	289	THR	C-O	6.34	1.31	1.24
1	D	498	ALA	N-CA	6.33	1.54	1.46
1	D	150	MET	N-CA	6.32	1.54	1.46
2	E	321	ALA	CA-CB	6.30	1.64	1.53
1	A	173	ALA	C-O	6.29	1.31	1.24
1	A	450	ASP	CA-CB	-6.25	1.43	1.53
1	A	203	GLY	N-CA	6.24	1.52	1.45
3	C	155	VAL	CA-CB	6.23	1.62	1.54
1	D	462	GLY	N-CA	6.19	1.54	1.45
2	E	85	ILE	N-CA	6.19	1.53	1.46
1	D	351	LYS	CA-C	6.17	1.60	1.52
1	A	254	ALA	N-CA	6.17	1.53	1.46
1	A	4[A]	LYS	N-CA	6.17	1.53	1.45
1	A	4[B]	LYS	N-CA	6.17	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	190	GLN	N-CA	6.15	1.54	1.46
3	C	230	ALA	N-CA	6.14	1.53	1.46
3	F	92	TYR	N-CA	6.14	1.54	1.46
2	E	348	ASP	CA-CB	6.11	1.62	1.53
1	A	236	ILE	C-O	6.10	1.31	1.24
1	D	450	ASP	CA-CB	-6.07	1.43	1.53
1	D	116	ILE	CA-C	6.07	1.60	1.52
3	F	218	ARG	CZ-NH1	6.06	1.41	1.32
2	E	415	ILE	CA-CB	6.04	1.62	1.54
2	B	212	ALA	C-O	6.04	1.31	1.24
2	B	338	ILE	C-O	6.01	1.31	1.24
3	F	85	ILE	CA-C	6.00	1.60	1.52
2	B	159	ALA	CA-CB	5.96	1.63	1.53
3	F	162	LEU	N-CA	5.95	1.53	1.45
3	F	60	ASP	CA-C	5.92	1.60	1.52
1	D	485	GLN	N-CA	5.91	1.53	1.46
3	F	147	ARG	N-CA	5.91	1.53	1.46
3	F	103	ARG	CA-CB	5.90	1.62	1.53
1	D	135	THR	CA-C	5.88	1.60	1.52
2	B	208	THR	C-O	5.87	1.30	1.24
2	E	437	ALA	N-CA	5.87	1.53	1.46
3	C	143	PHE	C-O	5.86	1.31	1.24
3	C	184	VAL	CA-CB	5.86	1.62	1.54
1	D	131	HIS	CA-C	5.84	1.60	1.52
1	A	60	ILE	CA-C	5.82	1.59	1.52
1	A	375	THR	N-CA	5.81	1.53	1.46
2	E	145	GLU	C-O	5.80	1.30	1.24
3	F	230	ALA	N-CA	5.80	1.53	1.46
3	F	154	SER	C-O	5.79	1.32	1.23
1	D	354	VAL	CA-CB	5.77	1.61	1.54
1	D	237	SER	C-O	5.77	1.31	1.24
1	A	309	ALA	C-O	5.75	1.30	1.24
3	F	39	ILE	N-CA	5.75	1.53	1.46
1	A	212	THR	C-O	5.71	1.30	1.24
3	F	133	ILE	C-O	5.70	1.30	1.24
2	B	111	ARG	CD-NE	5.69	1.54	1.46
1	A	401	ARG	CZ-NH1	5.69	1.40	1.32
1	A	131	HIS	CA-C	5.69	1.60	1.52
1	A	342	ILE	CA-CB	-5.68	1.47	1.54
2	B	284	VAL	C-O	5.68	1.29	1.24
1	D	19	GLU	CD-OE1	5.67	1.36	1.25
1	D	543	ARG	CB-CG	5.67	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	173	ARG	N-CA	5.66	1.54	1.46
2	E	272	LEU	CA-CB	5.66	1.62	1.53
2	B	23	PRO	CA-C	5.61	1.59	1.52
2	E	139	VAL	CA-CB	5.60	1.60	1.54
1	A	117	GLU	N-CA	5.59	1.53	1.46
2	B	63	GLY	N-CA	5.59	1.52	1.45
1	D	450	ASP	CA-C	-5.58	1.45	1.52
1	A	115	VAL	C-O	5.57	1.30	1.24
3	C	189	ASN	N-CA	5.56	1.52	1.45
1	D	394	ASP	CA-C	5.54	1.59	1.52
2	E	201	VAL	CA-CB	-5.53	1.47	1.54
1	D	299	ASP	N-CA	5.53	1.53	1.46
3	C	174	ARG	NE-CZ	5.52	1.39	1.33
2	E	426	ARG	N-CA	-5.49	1.39	1.46
1	D	261	ILE	CG1-CD1	-5.48	1.30	1.51
2	E	293	VAL	N-CA	5.46	1.53	1.46
1	A	514	ALA	CA-CB	5.46	1.59	1.52
1	A	545	LEU	C-O	5.44	1.31	1.24
2	B	82	ALA	CA-CB	-5.44	1.44	1.53
1	A	286	LEU	CA-CB	5.42	1.61	1.53
3	F	72	PRO	C-O	5.42	1.29	1.23
3	F	223	ALA	CA-C	-5.42	1.45	1.52
2	B	112	ALA	C-O	5.41	1.30	1.23
2	B	84	SER	CA-C	5.40	1.59	1.52
1	D	110	ASN	C-O	5.38	1.30	1.24
1	D	479	ALA	N-CA	5.37	1.53	1.46
2	E	168	VAL	N-CA	5.37	1.52	1.46
1	A	116	ILE	CA-CB	-5.35	1.48	1.54
2	B	111	ARG	C-O	5.35	1.30	1.23
2	B	78	ILE	CA-CB	5.35	1.60	1.54
1	D	414	ALA	CA-CB	5.34	1.62	1.53
1	A	129	ILE	N-CA	5.34	1.52	1.46
2	E	90	LYS	CA-CB	5.33	1.61	1.53
2	B	283	LYS	N-CA	5.32	1.52	1.45
2	B	241	LEU	CA-CB	5.31	1.61	1.53
1	D	440	ARG	N-CA	5.31	1.52	1.46
3	C	38	LYS	CA-CB	5.31	1.61	1.53
2	E	212	ALA	C-O	5.30	1.30	1.24
3	C	175	GLN	N-CA	5.30	1.52	1.46
3	F	126	ARG	C-O	5.29	1.30	1.23
2	E	230	VAL	CA-C	5.29	1.58	1.52
1	D	205	TRP	N-CA	5.28	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	137	ALA	N-CA	5.28	1.52	1.46
2	E	208	THR	N-CA	5.28	1.52	1.46
2	E	82	ALA	CA-C	-5.27	1.46	1.52
3	C	3	GLN	CB-CG	-5.27	1.36	1.52
3	C	153	LYS	CE-NZ	5.26	1.65	1.49
1	D	114	ALA	N-CA	5.26	1.52	1.46
1	D	146	VAL	CA-C	-5.25	1.47	1.52
1	A	92	ALA	C-N	5.25	1.40	1.33
1	D	380	TYR	N-CA	-5.25	1.40	1.46
1	A	281	VAL	N-CA	5.25	1.50	1.46
2	E	398	ALA	N-CA	5.25	1.52	1.46
3	C	226	ASP	N-CA	5.25	1.53	1.46
1	D	362	GLU	N-CA	5.25	1.52	1.46
1	A	90	ASN	N-CA	5.24	1.52	1.46
1	A	9	ALA	CA-CB	5.23	1.61	1.53
3	F	114	ALA	C-O	5.23	1.30	1.23
1	A	308	VAL	CA-C	5.22	1.59	1.52
2	E	198	ASN	N-CA	5.22	1.52	1.46
1	D	211	PRO	N-CA	5.22	1.53	1.47
1	A	130	THR	CA-C	5.18	1.59	1.52
1	D	281	VAL	N-CA	5.18	1.52	1.46
1	D	396	PHE	C-N	5.18	1.37	1.33
3	F	193	ASP	N-CA	5.18	1.52	1.46
1	D	223	THR	N-CA	5.18	1.52	1.46
1	A	20	GLU	C-O	5.17	1.30	1.23
2	E	311	MET	N-CA	5.17	1.52	1.46
3	C	60	ASP	CA-C	5.16	1.59	1.53
1	D	235	MET	N-CA	5.16	1.52	1.46
1	D	441	LEU	N-CA	5.15	1.52	1.46
2	E	112	ALA	C-O	5.14	1.29	1.23
2	E	75	ASP	C-O	5.14	1.29	1.23
1	D	497	ALA	CA-CB	5.13	1.61	1.53
1	A	125	THR	CA-CB	5.13	1.60	1.53
2	B	331	LEU	N-CA	5.13	1.52	1.46
3	C	95	PRO	CA-C	5.13	1.59	1.52
1	A	503	PHE	N-CA	5.13	1.52	1.46
3	F	27	LYS	C-O	5.13	1.30	1.24
3	C	224	TYR	CA-CB	5.12	1.61	1.53
3	F	11	VAL	N-CA	5.12	1.52	1.46
2	B	241	LEU	N-CA	-5.12	1.40	1.46
2	E	240	GLY	N-CA	5.11	1.52	1.45
2	B	188	PRO	C-O	5.10	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	TRP	N-CA	5.10	1.52	1.46
2	B	175	ILE	C-O	5.10	1.29	1.23
2	E	35	ILE	N-CA	5.10	1.52	1.46
1	A	386	GLU	N-CA	5.09	1.52	1.46
3	C	97	GLN	CA-C	5.08	1.57	1.52
1	D	94	MET	C-O	5.07	1.29	1.24
1	D	460	ILE	CA-CB	5.07	1.60	1.54
2	E	109	GLY	CA-C	5.07	1.58	1.51
3	C	218	ARG	CZ-NH1	5.07	1.39	1.32
2	E	5	GLU	N-CA	5.07	1.52	1.46
3	C	158	HIS	CA-CB	5.06	1.61	1.53
2	E	29	PRO	CA-CB	5.06	1.60	1.53
1	A	150	MET	C-O	5.05	1.30	1.23
3	C	63	GLU	CA-C	5.04	1.58	1.52
1	A	210	ILE	CA-C	5.03	1.58	1.52
2	E	96	THR	N-CA	5.03	1.52	1.45
1	D	349	PHE	CA-C	-5.02	1.46	1.52
2	B	338	ILE	CA-CB	-5.02	1.47	1.54
1	A	57	ASN	N-CA	5.02	1.53	1.46
1	D	149	HIS	CA-C	5.01	1.59	1.53
1	D	242	ALA	CA-CB	5.01	1.61	1.53
1	A	514	ALA	CA-C	-5.01	1.48	1.53
2	E	69	ILE	N-CA	5.01	1.53	1.46
2	B	437	ALA	C-O	5.01	1.30	1.24
2	B	36	LYS	C-O	5.01	1.29	1.24
2	B	2	ALA	N-CA	5.01	1.55	1.46

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	61	GLU	CA-C-N	-7.97	112.56	120.21
3	F	61	GLU	C-N-CA	-7.97	112.56	120.21
2	B	273	VAL	O-C-N	7.67	129.31	121.87
1	D	293	SER	CA-C-O	-7.39	112.65	120.63
1	A	450	ASP	CB-CA-C	7.15	122.66	110.79
1	D	538	GLU	CB-CA-C	-7.12	103.06	110.33
1	A	450	ASP	N-CA-CB	7.04	120.47	110.12
1	D	135	THR	O-C-N	6.67	129.29	122.09
1	D	97	MET	N-CA-C	-6.49	104.20	111.28
1	A	128	THR	N-CA-C	-6.46	104.32	111.82
3	F	54	PRO	N-CA-C	6.27	118.34	110.70
1	D	547	THR	O-C-N	6.24	126.62	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	335	ASN	N-CA-C	6.21	118.12	111.36
3	C	97	GLN	N-CA-C	-6.17	101.05	108.14
1	D	450	ASP	N-CA-CB	6.12	119.64	110.22
3	F	66	ILE	N-CA-C	6.05	116.23	110.42
1	A	60	ILE	CB-CA-C	-5.98	103.50	110.91
1	D	337	ALA	CA-C-O	-5.92	112.42	119.35
2	E	418	VAL	N-CA-C	5.89	116.54	110.82
2	B	383	ARG	N-CA-C	-5.87	106.11	113.28
2	E	32	ASN	O-C-N	-5.84	116.34	121.31
1	A	117	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	188	PHE	O-C-N	5.80	127.12	121.66
2	B	230	VAL	O-C-N	-5.78	116.94	123.18
3	F	217	TYR	O-C-N	-5.72	116.70	123.22
1	D	146	VAL	N-CA-CB	-5.68	106.99	111.64
3	F	144	ASP	O-C-N	-5.65	116.36	121.39
1	D	450	ASP	CB-CA-C	5.63	121.05	110.63
3	F	177	TYR	O-C-N	5.63	129.62	123.04
3	C	59	MET	N-CA-C	5.60	120.24	112.90
1	D	7	ILE	N-CA-C	5.58	116.31	110.62
1	D	486	GLY	N-CA-C	-5.54	105.95	113.37
2	B	242	ALA	CA-C-O	-5.54	115.00	120.70
1	D	477	ASN	CB-CG-ND2	5.50	124.65	116.40
1	A	21	LYS	N-CA-C	5.48	120.03	113.23
2	B	329	SER	CA-C-O	-5.46	115.08	120.70
1	A	10	LEU	O-C-N	5.45	127.90	122.12
2	B	440	LYS	CA-C-N	-5.42	114.01	122.73
2	B	440	LYS	C-N-CA	-5.42	114.01	122.73
3	C	147	ARG	NE-CZ-NH1	5.41	126.91	121.50
3	C	177	TYR	CA-C-N	-5.40	115.82	122.84
3	C	177	TYR	C-N-CA	-5.40	115.82	122.84
2	E	35	ILE	O-C-N	-5.38	116.65	121.87
2	B	333	TYR	CA-C-O	-5.38	112.64	119.31
1	D	306	ASP	N-CA-C	-5.37	105.51	111.36
1	A	128	THR	N-CA-CB	5.34	118.56	110.28
1	A	51	ARG	N-CA-C	5.30	119.75	113.28
3	F	236	ARG	O-C-N	5.29	127.52	122.07
1	A	242	ALA	N-CA-C	-5.29	102.56	110.23
2	B	286	LYS	N-CA-C	-5.27	100.72	108.99
1	A	117	GLU	CA-CB-CG	-5.24	103.63	114.10
2	E	329	SER	N-CA-CB	-5.23	102.42	110.16
1	D	345	ASP	CA-C-O	5.21	126.30	120.82
2	B	361	PHE	CA-C-O	-5.21	115.35	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLY	O-C-N	5.18	127.64	122.92
1	D	235	MET	N-CA-C	-5.15	105.75	111.36
2	E	18	VAL	N-CA-C	-5.15	107.13	111.56
2	B	418	VAL	N-CA-C	5.12	116.21	111.45
1	A	70	MET	CB-CA-C	-5.11	101.50	108.86
1	A	13	LYS	N-CA-C	5.08	117.94	111.69
1	D	213	ILE	CA-C-O	-5.08	114.99	120.47
3	F	59	MET	CG-SD-CE	-5.08	89.73	100.90
1	D	394	ASP	N-CA-C	-5.07	105.40	111.03
1	A	375	THR	CA-C-O	-5.06	115.49	120.70
1	D	525	VAL	CA-C-O	-5.06	115.81	121.17
1	A	305	LEU	CA-C-N	-5.05	113.51	120.28
1	A	305	LEU	C-N-CA	-5.05	113.51	120.28
1	A	513	PHE	O-C-N	5.04	128.25	122.25
1	A	480	MET	CA-C-N	-5.01	114.94	122.81
1	A	480	MET	C-N-CA	-5.01	114.94	122.81
1	A	549	ALA	CA-C-O	-5.01	112.28	120.80
1	D	70	MET	CB-CA-C	-5.01	101.65	108.86
3	F	11	VAL	O-C-N	-5.01	117.00	121.91

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

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	4241	31	0
1	D	4390	0	4229	27	0
2	B	3505	0	3572	40	0
2	E	3519	0	3563	38	0
3	C	2050	0	1984	25	0
3	F	2103	0	2051	28	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	7	0
13	B	472	0	0	17	0
13	C	259	0	0	5	0
13	D	511	0	0	7	0
13	E	415	0	0	13	0
13	F	256	0	0	11	0
All	All	22789	0	19918	174	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 (174) 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:HG2	3:F:67[A]:ARG:HH11	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
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	1.95	0.97
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.45	0.94
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
3:F:67[A]:ARG:HG2	3:F:67[A]:ARG:NH1	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
2:B:196[B]:MET:HE1	13:B:574:HOH:O	1.89	0.72
2:B:322[B]:ARG:CZ	3:C:67[B]:ARG:HG3	2.22	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
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
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:B:196[B]:MET:CE	13:B:574:HOH:O	2.42	0.65
1:A:24[B]:THR:HG23	13:A:677:HOH:O	1.96	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:D:268:PRO:HB3	13:E:1668:HOH:O	2.02	0.59
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
1:A:357:LYS:NZ	1:A:372[B]:ASP:OD1	2.32	0.57
2:B:95:VAL:HG21	2:B:119[B]:ALA:HB3	1.87	0.57
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
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.73	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:4[A]:LYS:NZ	13:A:2253:HOH:O	2.32	0.54
1:A:17[B]:SER:OG	1:A:20:GLU:HG3	2.08	0.54
2:B:196[B]:MET:HE2	13:B:3731:HOH:O	2.07	0.53
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:42[A]:ILE:HG13	2:B:425:PHE:CE1	2.44	0.52
2:B:424[A]:GLU:HG3	13:B:3930:HOH:O	2.08	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:D:358:TYR:OH	1:D:372[A]:ASP:OD2	2.25	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
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.45	0.51
3:F:247:ASN:C	3:F:247:ASN:HD22	2.18	0.51
2:E:299:LEU:HD22	13:E:2973:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:27:LEU:HD21	2:E:246[B]:MET:HE1	1.88	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
3:F:59:MET:O	3:F:60:ASP:C	2.56	0.47
10:F:251:EDO:C2	13:F:832:HOH:O	2.63	0.47
1:A:383[A]:GLU:HG3	13:A:2606:HOH:O	2.15	0.47
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:A:186:LYS:HB2	1:A:186:LYS:NZ	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:A:448:LEU:O	1:A:452:SMC:HCS3	2.17	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
2:B:246[A]:MET:HE3	2:B:429:LEU:HD12	1.99	0.44
1:A:115:VAL:CG2	2:E:405[B]:MET:SD	3.06	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:172:ILE:CD1	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:B:61[B]:LYS:NZ	13:B:1223:HOH:O	2.36	0.43
2:E:39:VAL:HG21	2:E:221:THR:HG21	2.01	0.43
2:B:113[B]:LEU:HD23	2:B:113[B]:LEU:C	2.44	0.43
2:E:374:ILE:C	2:E:374:ILE:HD12	2.44	0.43
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	2.01	0.42
1:D:169:ASN:CG	1:D:172[A]:ILE:HG13	2.44	0.42
2:E:61[B]:LYS:CE	13:E:2444:HOH:O	2.66	0.42
2:E:113[A]:LEU:HD13	2:E:418:VAL:HG13	2.00	0.42
13:E:3631[A]:HOH:O	3:F:72:PRO:HG3	2.18	0.42
2:B:3:LYS:HZ2	2:B:3:LYS:HG3	1.67	0.42
2:B:322[B]:ARG:HH21	3:C:67[B]:ARG:CG	2.22	0.42
3:F:116:THR:C	3:F:117:LEU:HD12	2.45	0.42
1:D:448:LEU:O	1:D:452:SMC:HCS3	2.20	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
1:A:443:PHE:CZ	6:A:553[A]:TP7:S7	3.13	0.41
3:C:100:VAL:HG21	3:C:215:THR:HB	2.03	0.41
2:E:208:THR:HG22	2:E:315:MET:HE2	2.03	0.41
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.51	0.41
2:E:424[A]:GLU:HG2	13:E:3642:HOH:O	2.20	0.41
2:B:126:GLU:HB3	2:E:126:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:555[B]:XP9:H7A	2:E:361:PHE:HE2	1.85	0.41
2:E:261:LYS:HG2	13:F:3664:HOH:O	2.20	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
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/549 (105%)	556 (97%)	17 (3%)	1 (0%)	43	21
1	D	566/549 (103%)	549 (97%)	16 (3%)	1 (0%)	43	21
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%)	30	11
All	All	2600/2478 (105%)	2528 (97%)	69 (3%)	3 (0%)	48	22

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 ⓘ

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%)	455 (98%)	11 (2%)	43	12
1	D	458/434 (106%)	457 (100%)	1 (0%)	87	76
2	B	371/341 (109%)	365 (98%)	6 (2%)	55	23
2	E	372/341 (109%)	365 (98%)	7 (2%)	50	17
3	C	224/216 (104%)	220 (98%)	4 (2%)	51	19
3	F	232/216 (107%)	220 (95%)	12 (5%)	21	2
All	All	2123/1982 (107%)	2082 (98%)	41 (2%)	55	17

All (41) 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	186	LYS
1	A	450	ASP
2	B	3	LYS
2	B	97	GLU
2	B	123[A]	VAL
2	B	123[B]	VAL
2	B	283	LYS
2	B	287	GLU
3	C	45	PRO
3	C	61	GLU
3	C	150	VAL
3	C	208	GLU
1	D	450	ASP

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Mol	Chain	Res	Type
2	E	236[A]	MET
2	E	236[B]	MET
2	E	236[C]	MET
2	E	283	LYS
2	E	374	ILE
2	E	438[A]	GLU
2	E	438[B]	GLU
3	F	57	GLU
3	F	60	ASP
3	F	61	GLU
3	F	67[A]	ARG
3	F	67[B]	ARG
3	F	117	LEU
3	F	121	GLN
3	F	150	VAL
3	F	186	MET
3	F	207[A]	GLU
3	F	207[B]	GLU
3	F	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	241	GLN
1	A	437	GLN
2	B	102	ASN
2	B	115	GLN
3	C	121	GLN
1	D	296	ASN
1	D	317	GLN
1	D	437	GLN
2	E	21	GLN
2	E	81	ASN
2	E	102	ASN
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	D	452	1	5,6,7	0.95	0	3,6,8	1.69	1 (33%)
1	MHS	A	257	1	10,11,12	2.57	4 (40%)	5,14,16	11.49	3 (60%)
1	GL3	D	445	1	2,3,4	2.02	1 (50%)	1,2,4	0.40	0
1	AGM	D	271	1	10,11,12	1.70	2 (20%)	7,13,15	1.51	1 (14%)
1	MHS	D	257	1	10,11,12	1.87	2 (20%)	5,14,16	9.13	4 (80%)
1	MGN	A	400	1	6,9,10	1.08	0	7,12,14	1.10	1 (14%)
1	GL3	A	445	1	2,3,4	2.03	1 (50%)	1,2,4	0.23	0
1	SMC	A	452	1	5,6,7	1.20	0	3,6,8	1.95	1 (33%)
1	MGN	D	400	1	6,9,10	1.45	1 (16%)	7,12,14	1.03	1 (14%)
1	AGM	A	271	1	10,11,12	1.39	2 (20%)	7,13,15	2.05	3 (42%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CE1-NE2	4.59	1.44	1.32
1	A	257	MHS	CG-ND1	-3.86	1.31	1.38
1	D	257	MHS	CE1-NE2	3.79	1.42	1.32
1	D	271	AGM	CB-CA	3.72	1.59	1.53
1	A	257	MHS	CE1-ND1	3.00	1.43	1.35
1	A	445	GL3	C-S	-2.88	1.68	1.80
1	D	445	GL3	C-S	-2.85	1.68	1.80
1	D	257	MHS	CE1-ND1	2.77	1.42	1.35
1	D	400	MGN	O-C	2.69	1.28	1.20
1	A	257	MHS	CB-CA	2.54	1.59	1.53
1	A	271	AGM	O-C	2.50	1.29	1.20
1	A	271	AGM	CZ-NH2	2.48	1.41	1.32
1	D	271	AGM	CZ-NH2	2.00	1.39	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	ND1-CE1-NE2	-24.81	98.17	112.94
1	D	257	MHS	ND1-CE1-NE2	-19.13	101.55	112.94
1	A	257	MHS	CD2-NE2-CE1	4.74	111.44	105.24
1	D	257	MHS	CD2-NE2-CE1	4.58	111.23	105.24
1	D	257	MHS	CM-ND1-CE1	-4.38	118.09	126.28
1	A	257	MHS	CM-ND1-CE1	-4.21	118.41	126.28
1	A	271	AGM	NE1-CZ-NH2	-3.43	114.70	120.58
1	A	452	SMC	CA-CB-SG	-3.19	108.89	114.04
1	D	257	MHS	CM-ND1-CG	3.07	129.96	126.69
1	A	271	AGM	NH1-CZ-NE1	2.78	125.72	119.58
1	D	271	AGM	NE1-CZ-NH2	-2.52	116.26	120.58
1	D	452	SMC	CA-CB-SG	-2.49	110.01	114.04
1	D	400	MGN	CB1-CA-C	-2.43	102.21	108.47
1	A	400	MGN	CB1-CG-CD	-2.35	107.44	112.13
1	A	271	AGM	CD-NE1-CZ	-2.21	119.47	123.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	A	445	GL3	S-C-CA-N
1	D	445	GL3	S-C-CA-N
1	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
8	XP9	A	555[C]	-	21,22,22	0.85	0	26,28,28	0.93	1 (3%)
7	COM	A	554	5	6,6,6	1.41	1 (16%)	8,8,8	1.52	3 (37%)
10	EDO	C	251	-	3,3,3	0.55	0	2,2,2	0.52	0
10	EDO	F	251	-	3,3,3	0.63	0	2,2,2	0.61	0
8	XP9	D	555[C]	-	21,22,22	0.82	1 (4%)	26,28,28	0.96	1 (3%)
10	EDO	A	557	-	3,3,3	0.79	0	2,2,2	0.63	0
6	TP7	A	553[A]	-	19,20,20	1.16	2 (10%)	24,26,26	1.07	1 (4%)
8	XP9	A	555[B]	-	21,22,22	0.89	0	26,28,28	1.20	2 (7%)
10	EDO	D	556	-	3,3,3	0.46	0	2,2,2	0.57	0
5	F43	D	552	1,7	63,71,71	2.56	14 (22%)	73,118,118	2.01	16 (21%)
8	XP9	D	555[B]	-	21,22,22	0.85	1 (4%)	26,28,28	1.09	2 (7%)
10	EDO	F	252	-	3,3,3	0.75	0	2,2,2	0.18	0
9	ACT	A	556[B]	4	3,3,3	0.52	0	3,3,3	1.60	1 (33%)
10	EDO	B	446	-	3,3,3	0.49	0	2,2,2	0.36	0
5	F43	A	1	1,7	63,71,71	2.56	14 (22%)	73,118,118	1.61	14 (19%)
6	TP7	D	553[A]	-	19,20,20	1.19	2 (10%)	24,26,26	1.06	2 (8%)
12	PEG	C	252	-	6,6,6	0.58	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	COM	D	554	5	6,6,6	0.85	0	8,8,8	1.05	0
9	ACT	C	1	-	3,3,3	0.46	0	3,3,3	2.01	1 (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
7	COM	A	554	5	-	0/4/4/4	-
10	EDO	B	446	-	-	1/1/1/1	-
10	EDO	C	251	-	-	0/1/1/1	-
8	XP9	D	555[B]	-	-	4/26/26/26	-
5	F43	A	1	1,7	-	10/28/185/185	-
8	XP9	D	555[C]	-	-	1/26/26/26	-
10	EDO	F	251	-	-	1/1/1/1	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	F	252	-	-	1/1/1/1	-
6	TP7	D	553[A]	-	-	0/24/24/24	-
6	TP7	A	553[A]	-	-	2/24/24/24	-
12	PEG	C	252	-	-	1/4/4/4	-
7	COM	D	554	5	-	0/4/4/4	-
8	XP9	A	555[B]	-	-	3/26/26/26	-
10	EDO	D	556	-	-	1/1/1/1	-
8	XP9	A	555[C]	-	-	3/26/26/26	-
5	F43	D	552	1,7	-	9/28/185/185	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	NI-NB	9.89	2.13	1.89
5	D	552	F43	NI-NA	9.50	2.12	1.89
5	A	1	F43	NI-NA	9.42	2.12	1.89
5	D	552	F43	NI-NB	9.15	2.11	1.89
5	A	1	F43	NI-ND	7.87	2.08	1.89
5	D	552	F43	NI-ND	7.26	2.07	1.89
5	D	552	F43	CHB-C1B	5.07	1.56	1.53
5	D	552	F43	CHD-C1D	4.43	1.50	1.43
5	D	552	F43	C3C-C4C	4.24	1.57	1.50
5	A	1	F43	CHC-C4B	4.07	1.50	1.39
5	A	1	F43	CHA-C4D	3.88	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	C3C-C4C	3.88	1.56	1.50
5	D	552	F43	O8D-C7D	3.45	1.30	1.23
5	A	1	F43	CHB-C4A	3.16	1.56	1.51
5	A	1	F43	OEB-CCB	-2.97	1.21	1.30
5	D	552	F43	C5C-C2C	2.96	1.58	1.53
5	A	1	F43	C4A-NA	2.87	1.53	1.49
6	D	553[A]	TP7	P-O4P	2.83	1.64	1.59
5	D	552	F43	OEB-CCB	-2.83	1.21	1.30
7	A	554	COM	C2-S2	2.83	1.81	1.77
5	A	1	F43	C8B-C6B	2.70	1.56	1.50
5	D	552	F43	C1C-NC	2.65	1.43	1.37
5	D	552	F43	CAA-CBA	2.60	1.60	1.52
5	A	1	F43	C9B-C2B	2.59	1.59	1.54
5	D	552	F43	CAA-C3A	2.54	1.58	1.53
5	D	552	F43	CHC-C4B	2.50	1.46	1.39
6	D	553[A]	TP7	OXT-C	2.46	1.29	1.22
8	D	555[C]	XP9	P-O4P	2.39	1.63	1.59
8	D	555[B]	XP9	P-O4P	2.37	1.63	1.59
6	A	553[A]	TP7	OXT-C	2.25	1.28	1.22
5	A	1	F43	O7C-C6C	2.25	1.29	1.22
5	A	1	F43	OCC-CAC	2.20	1.29	1.22
6	A	553[A]	TP7	P-O4P	2.15	1.63	1.59
5	A	1	F43	C5C-C2C	-2.10	1.49	1.53
5	D	552	F43	C2A-C3A	-2.06	1.51	1.54

All (44) 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	120.87
5	D	552	F43	C4B-CHC-C1C	5.70	135.06	125.84
5	D	552	F43	C6D-C7D-CHD	5.19	126.53	116.94
5	D	552	F43	C3A-C2A-C1A	4.46	104.43	99.97
5	D	552	F43	C5D-C2D-C1D	4.05	115.72	110.43
5	A	1	F43	O8D-C7D-C6D	-3.90	114.48	120.87
8	A	555[B]	XP9	C7-C8-C9	3.76	119.77	113.09
5	D	552	F43	C2D-C1D-CHD	-3.66	117.31	121.85
5	D	552	F43	C9A-C2A-C3A	3.57	118.12	112.99
5	A	1	F43	OBC-CAC-C9C	3.48	124.99	114.00
5	A	1	F43	C2C-C5C-C6C	-3.29	107.78	113.95
5	D	552	F43	C3D-C2D-C1D	-3.10	97.01	102.47
5	A	1	F43	C1B-C2B-C3B	3.08	105.99	101.51
5	A	1	F43	OCC-CAC-C9C	-3.02	113.51	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	F43	C9A-C2A-C3A	2.95	117.22	112.99
5	D	552	F43	O8C-C6C-C5C	2.91	123.06	114.00
6	A	553[A]	TP7	CB-CA-N	2.87	117.74	111.54
5	A	1	F43	CAB-C3B-C2B	-2.84	112.73	119.00
5	D	552	F43	C1D-CHD-C4C	-2.80	117.41	125.28
9	C	1	ACT	OXT-C-CH3	2.79	126.75	115.05
5	A	1	F43	C9B-C2B-C8B	-2.71	103.80	110.61
8	A	555[B]	XP9	CB-CA-N	2.59	117.14	111.54
5	D	552	F43	OBC-CAC-C9C	2.58	122.15	114.00
5	A	1	F43	C3A-C2A-C1A	-2.52	97.45	99.97
5	D	552	F43	CAB-C3B-C2B	-2.51	113.45	119.00
6	D	553[A]	TP7	CB-CA-N	2.50	116.95	111.54
8	D	555[B]	XP9	C7-C8-C9	2.49	117.51	113.09
8	A	555[C]	XP9	CB-CA-N	2.47	116.88	111.54
5	A	1	F43	ODB-CCB-CBB	-2.47	115.27	123.09
5	A	1	F43	C4A-NA-C1A	-2.46	105.73	109.08
5	D	552	F43	C2B-C1B-NB	2.45	105.50	101.86
7	A	554	COM	O3S-S2-O1S	2.43	117.47	111.40
8	D	555[B]	XP9	CB-CA-N	2.41	116.74	111.54
5	D	552	F43	C2C-C5C-C6C	-2.36	109.52	113.95
7	A	554	COM	O1S-S2-C2	-2.32	103.23	106.73
5	A	1	F43	C5D-C2D-C1D	2.24	113.35	110.43
6	D	553[A]	TP7	O4P-P-O1P	-2.18	101.57	109.33
8	D	555[C]	XP9	CB-CA-N	2.17	116.22	111.54
9	A	556[B]	ACT	OXT-C-CH3	2.15	124.07	115.05
5	D	552	F43	O7C-C6C-C5C	-2.15	116.24	122.84
5	D	552	F43	C7D-CHD-C4C	2.11	126.18	121.76
7	A	554	COM	O3S-S2-O2S	-2.09	106.16	111.40
5	A	1	F43	C3B-C4B-CHC	-2.06	118.94	123.33
5	A	1	F43	O7C-C6C-C5C	-2.03	116.59	122.84

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
8	D	555[B]	XP9	C4-C5-C6-C7
8	D	555[B]	XP9	C6-C7-C8-C9
10	D	556	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	F	252	EDO	O1-C1-C2-O2
10	A	557	EDO	O1-C1-C2-O2
10	B	446	EDO	O1-C1-C2-O2
8	D	555[B]	XP9	C2-C3-C4-C5
8	A	555[C]	XP9	C7-C8-C9-S9
8	D	555[C]	XP9	C7-C8-C9-S9
10	F	251	EDO	O1-C1-C2-O2
6	A	553[A]	TP7	CB-O4P-P-O3P
5	D	552	F43	C2C-C5C-C6C-O8C
5	A	1	F43	CAA-CBA-CCA-OEA
5	D	552	F43	CAA-CBA-CCA-OEA
5	A	1	F43	CAA-CBA-CCA-ODA
5	D	552	F43	CAB-CBB-CCB-OEB
5	A	1	F43	CAB-CBB-CCB-OEB
5	D	552	F43	CAA-CBA-CCA-ODA
8	A	555[C]	XP9	C2-C3-C4-C5
5	D	552	F43	C8C-C9C-CAC-OBC
5	A	1	F43	C8C-C9C-CAC-OCC
5	D	552	F43	CAB-CBB-CCB-ODB
5	A	1	F43	C3D-C9D-CAD-OCD
5	D	552	F43	C2C-C5C-C6C-O7C
5	A	1	F43	CAB-CBB-CCB-ODB
8	A	555[B]	XP9	CB-O4P-P-O3P
8	A	555[C]	XP9	CB-O4P-P-O3P
8	D	555[B]	XP9	CB-O4P-P-O3P
5	A	1	F43	C2C-C5C-C6C-O7C
5	A	1	F43	C3D-C9D-CAD-OB
5	A	1	F43	C8C-C9C-CAC-OBC
6	A	553[A]	TP7	C2-C3-C4-C5
12	C	252	PEG	O2-C3-C4-O4
5	D	552	F43	C3D-C9D-CAD-OCD

There are no ring outliers.

9 monomers are involved in 23 short contacts:

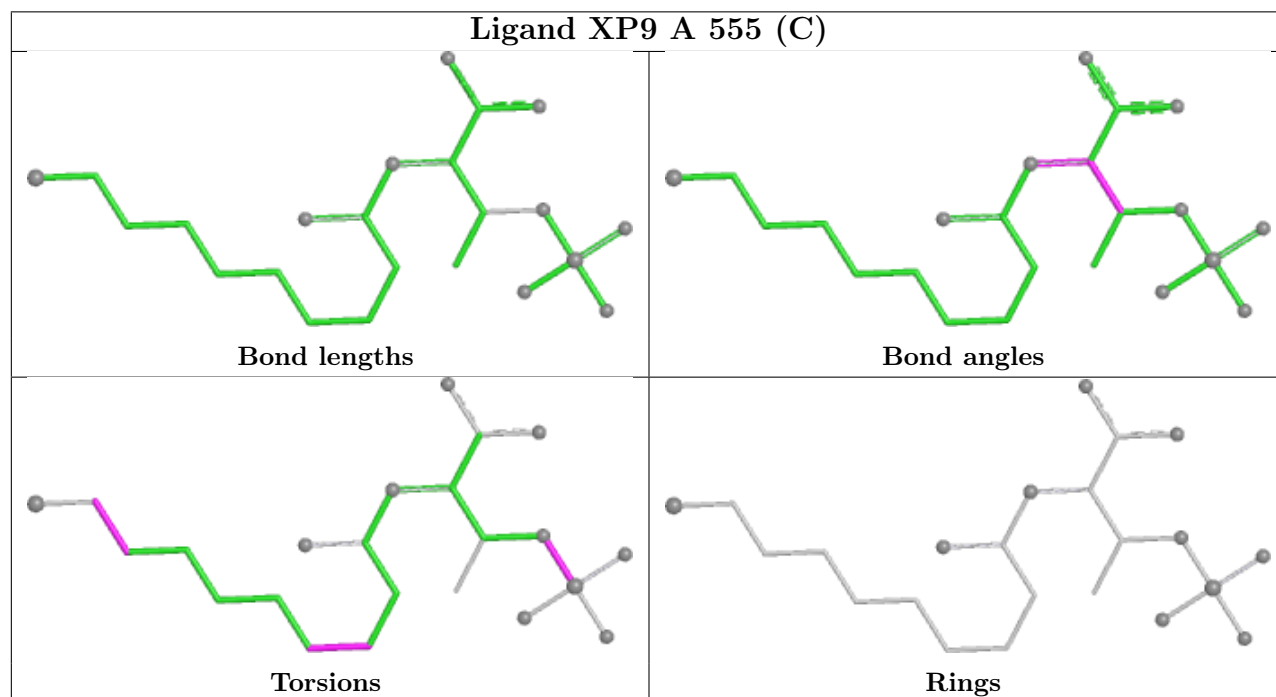
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	251	EDO	1	0
6	A	553[A]	TP7	2	0
8	A	555[B]	XP9	1	0
10	D	556	EDO	1	0
5	D	552	F43	1	0
8	D	555[B]	XP9	3	0

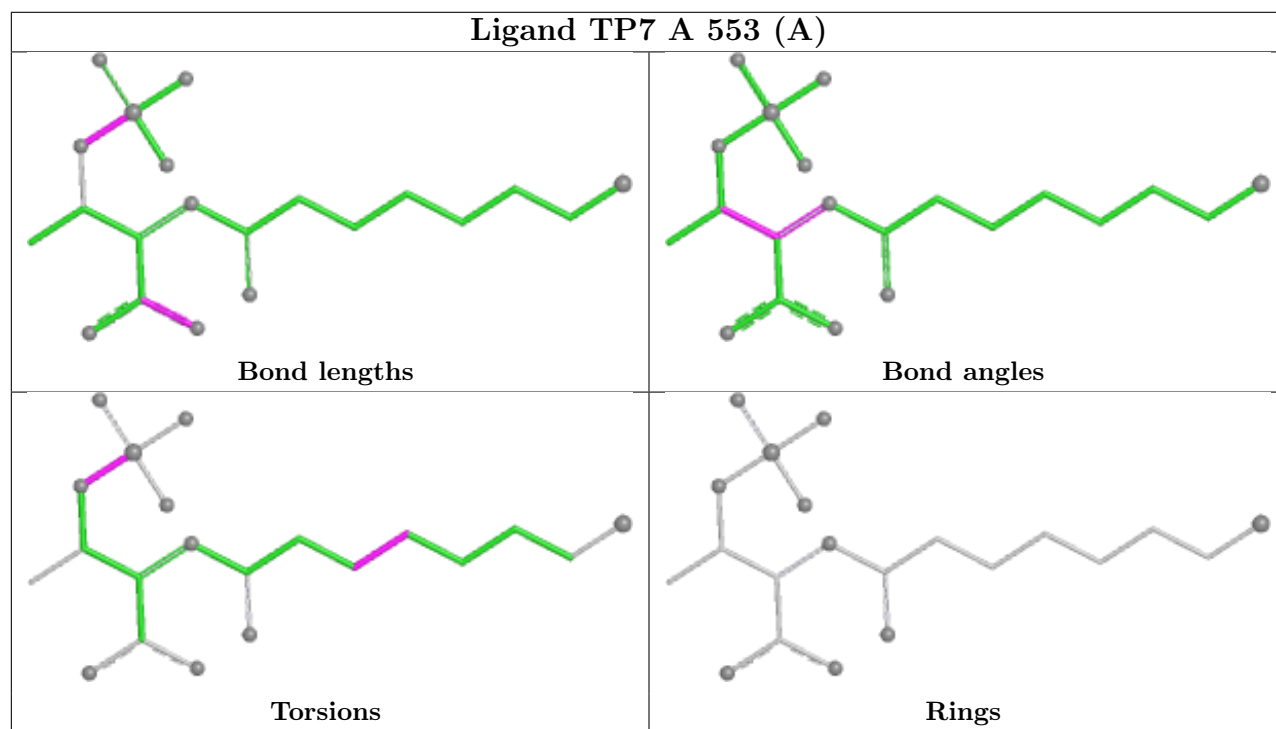
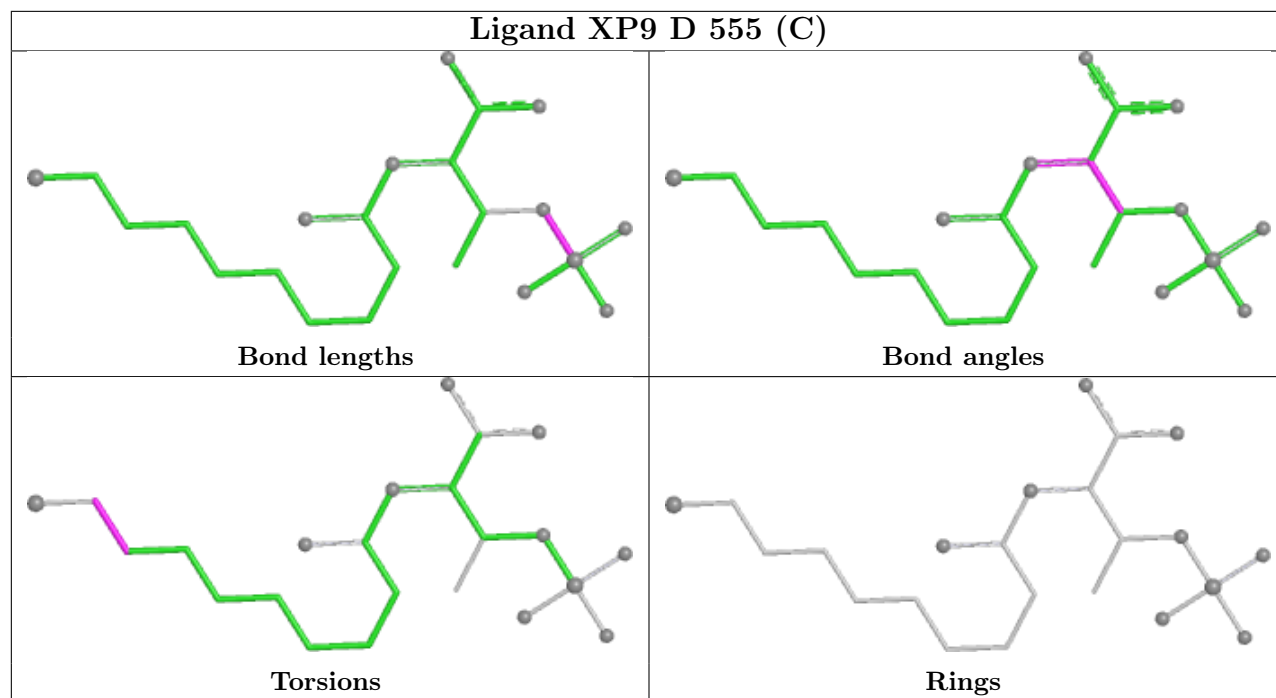
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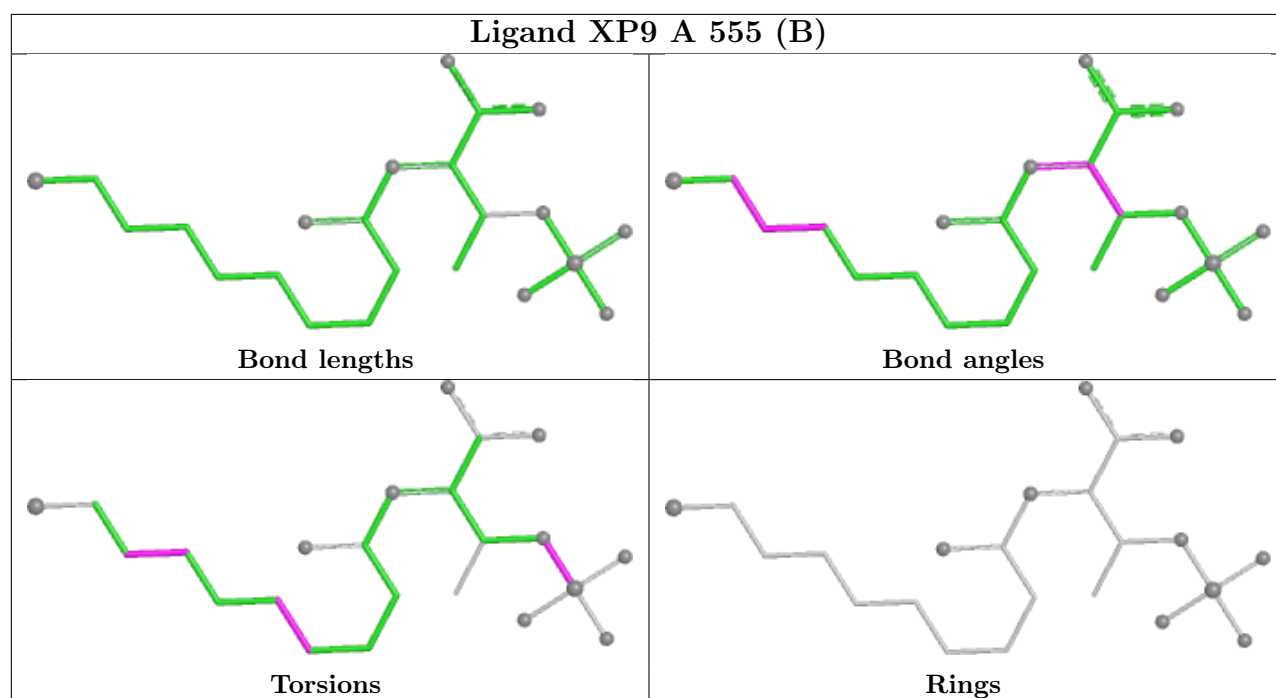
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	252	EDO	3	0
5	A	1	F43	1	0
9	C	1	ACT	10	0

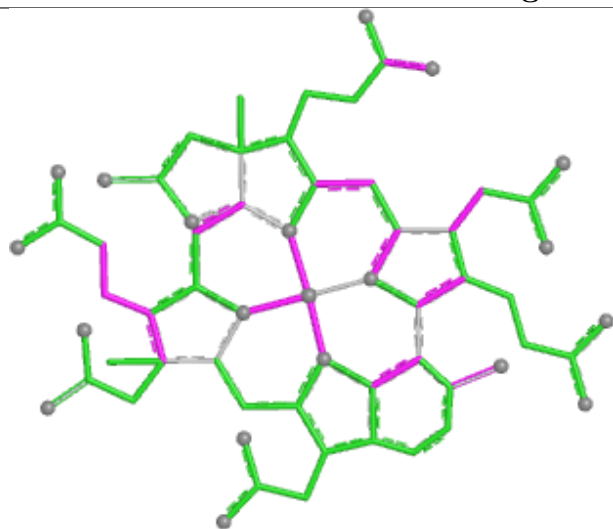
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



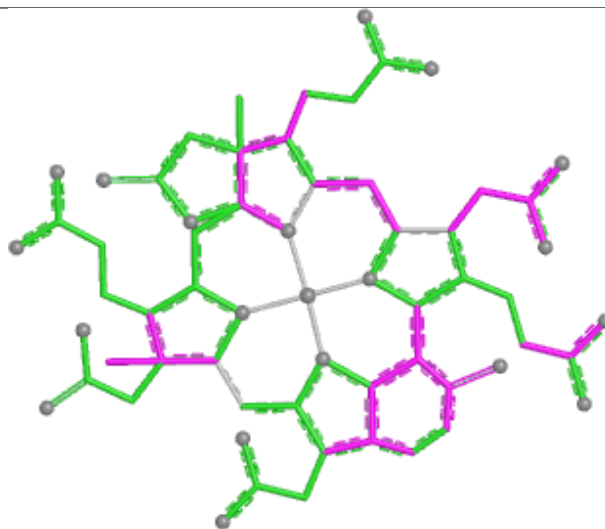




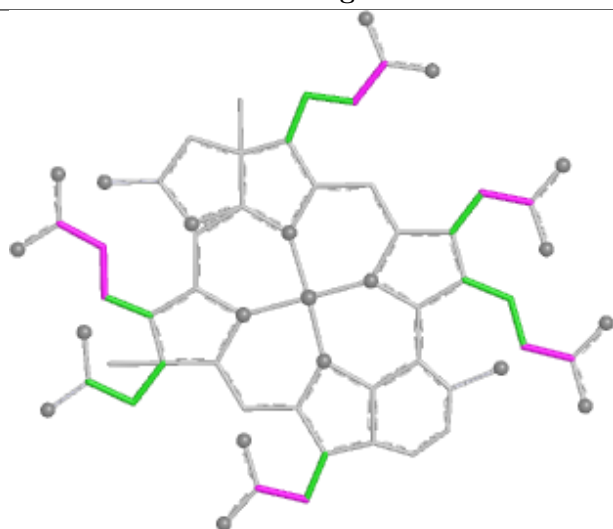
Ligand F43 D 552



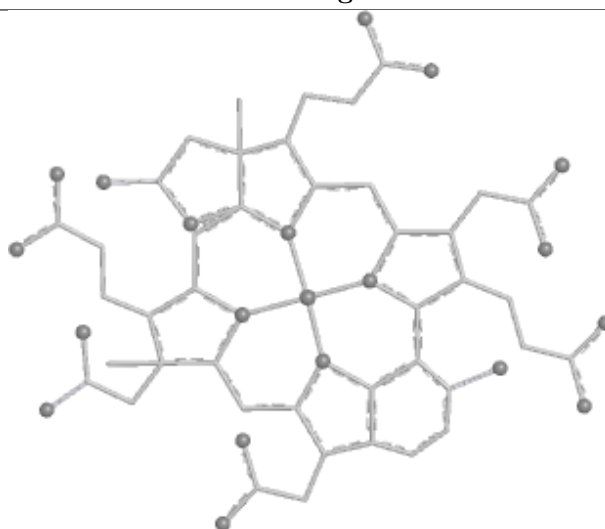
Bond lengths



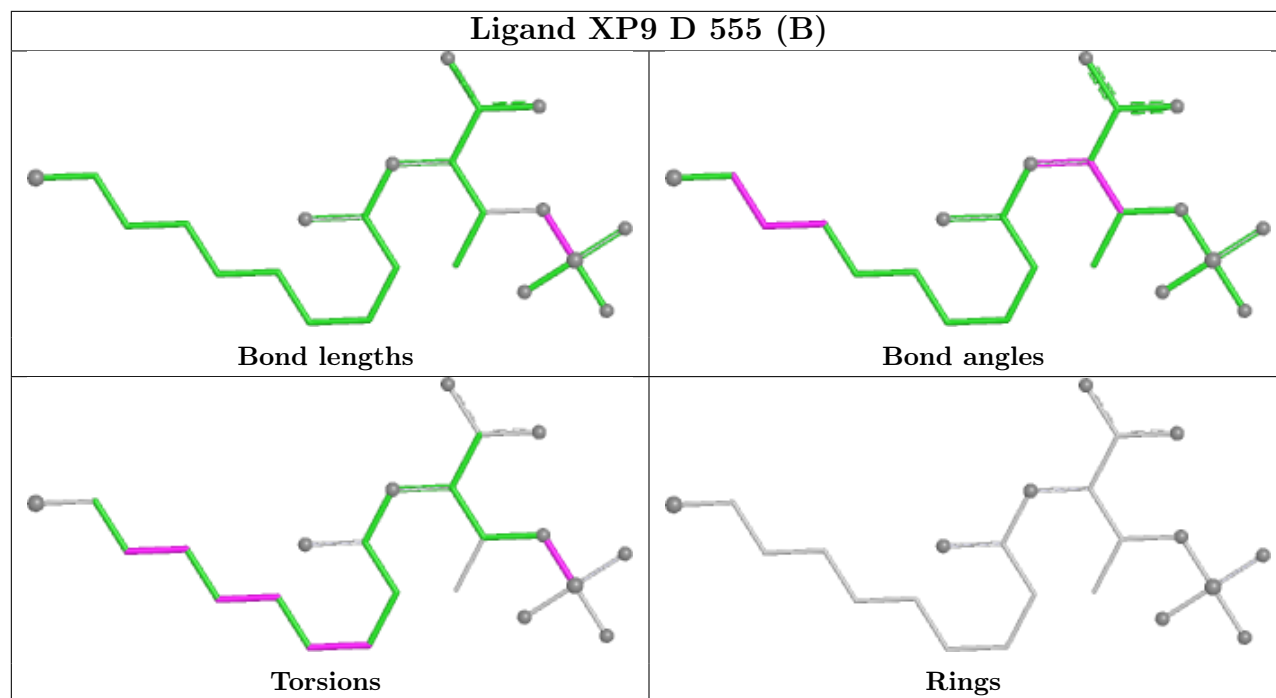
Bond angles



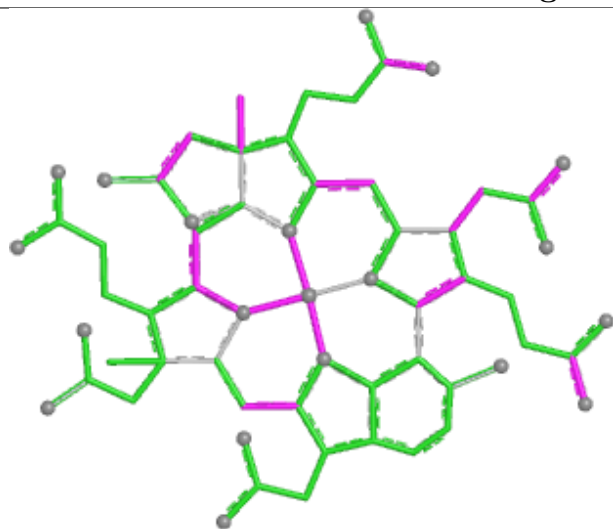
Torsions



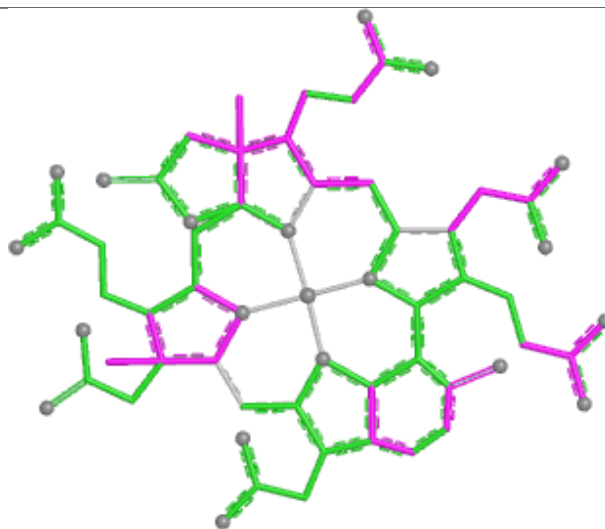
Rings



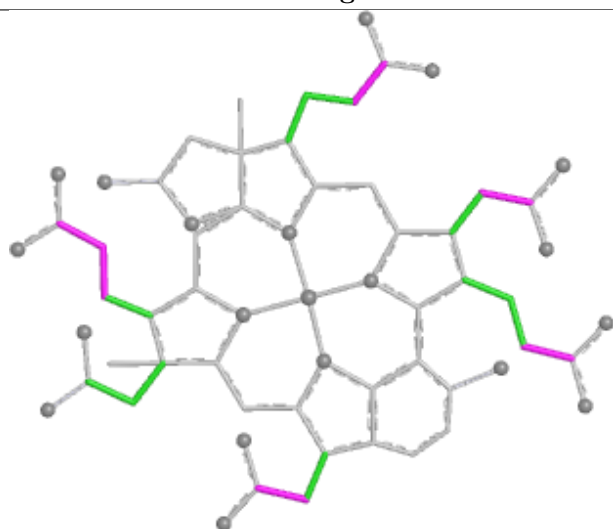
Ligand F43 A 1



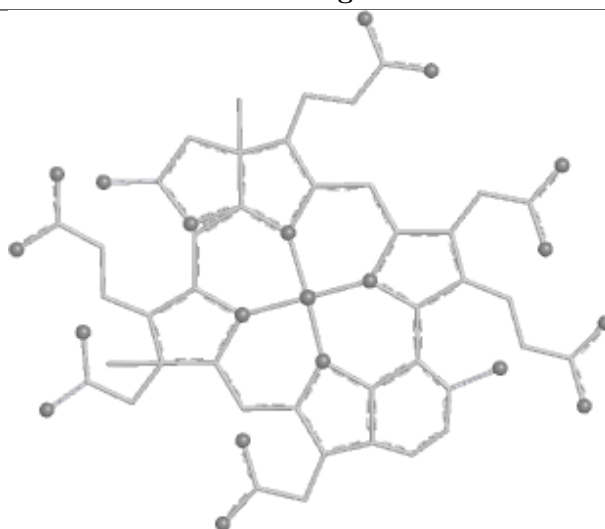
Bond lengths



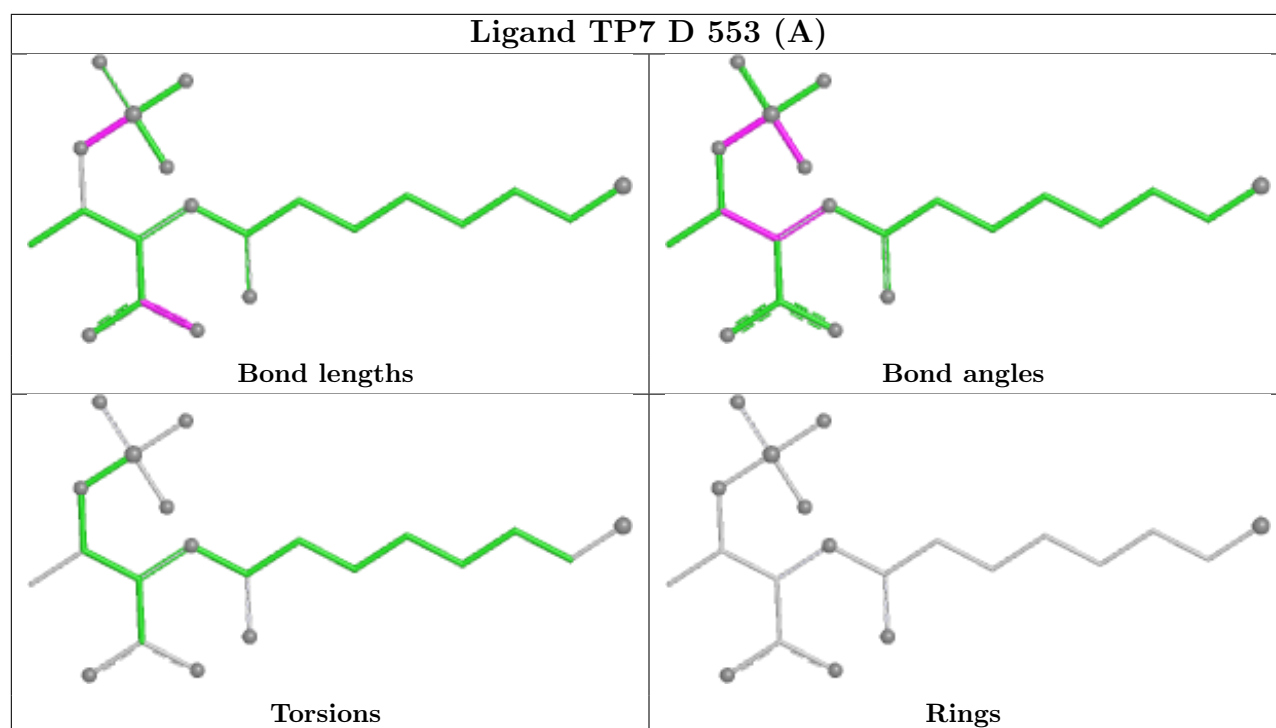
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/549 (98%)	-0.85	0 100 100	4, 9, 18, 34	32 (5%)
1	D	543/549 (98%)	-0.85	1 (0%) 91 93	4, 9, 20, 38	25 (4%)
2	B	442/442 (100%)	-0.79	1 (0%) 91 93	5, 11, 19, 39	30 (6%)
2	E	442/442 (100%)	-0.70	0 100 100	5, 12, 23, 42	31 (7%)
3	C	246/248 (99%)	-0.56	2 (0%) 82 86	5, 13, 30, 49	10 (4%)
3	F	246/248 (99%)	-0.50	2 (0%) 82 86	5, 13, 29, 53	19 (7%)
All	All	2462/2478 (99%)	-0.75	6 (0%) 91 93	4, 11, 22, 53	147 (5%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	45	PRO	2.5
2	B	98	ASP	2.2
3	C	59	MET	2.2
1	D	549	ALA	2.2
3	C	45	PRO	2.2
3	F	60	ASP	2.1

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	D	257	11/12	0.97	0.04	8,10,12,13	0
1	AGM	D	271	12/13	0.97	0.04	5,6,7,9	0
1	MHS	A	257	11/12	0.98	0.04	9,11,13,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MGN	A	400	10/11	0.98	0.04	5,7,8,8	0
1	AGM	A	271	12/13	0.99	0.03	5,6,7,8	0
1	SMC	A	452	7/8	0.99	0.04	6,7,8,10	0
1	MGN	D	400	10/11	0.99	0.03	6,7,8,8	0
1	SMC	D	452	7/8	0.99	0.04	7,7,10,11	0
1	GL3	D	445	4/5	1.00	0.02	5,6,6,7	0
1	GL3	A	445	4/5	1.00	0.03	5,6,7,7	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	EDO	C	251	4/4	0.83	0.11	36,39,40,43	0
9	ACT	C	1	4/4	0.84	0.15	27,29,30,33	4
10	EDO	F	252	4/4	0.84	0.11	35,39,40,44	0
10	EDO	F	251	4/4	0.85	0.10	34,34,36,39	0
10	EDO	A	557	4/4	0.86	0.10	35,35,36,43	0
12	PEG	C	252	7/7	0.87	0.11	37,38,44,44	0
10	EDO	D	556	4/4	0.88	0.10	33,36,41,41	0
10	EDO	B	446	4/4	0.88	0.11	42,42,43,44	0
9	ACT	A	556[B]	4/4	0.94	0.09	13,15,16,17	4
4	MG	B	445	1/1	0.95	0.20	34,34,34,34	0
4	MG	B	444	1/1	0.96	0.08	26,26,26,26	0
8	XP9	D	555[B]	23/23	0.98	0.04	6,7,10,12	23
8	XP9	D	555[C]	23/23	0.98	0.04	6,8,9,11	23
4	MG	A	551[A]	1/1	0.98	0.08	20,20,20,20	1
4	MG	A	552[B]	1/1	0.98	0.03	12,12,12,12	1
4	MG	C	250	1/1	0.98	0.06	15,15,15,15	0
4	MG	D	1	1/1	0.98	0.11	21,21,21,21	0
4	MG	E	444	1/1	0.98	0.10	21,21,21,21	0
4	MG	F	250	1/1	0.98	0.05	15,15,15,15	0
6	TP7	D	553[A]	21/21	0.98	0.04	7,8,9,12	21
8	XP9	A	555[B]	23/23	0.98	0.04	6,7,9,11	23

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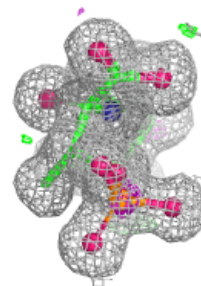
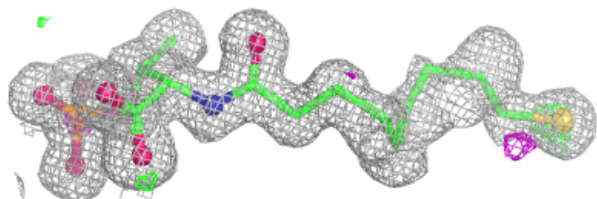
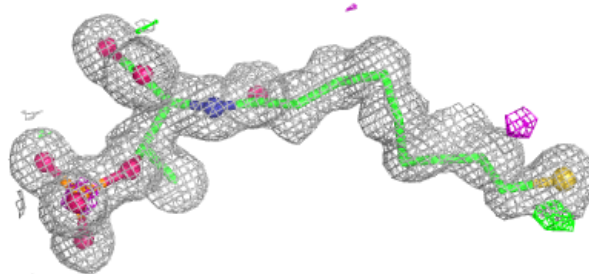
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	XP9	A	555[C]	23/23	0.98	0.04	5,8,8,10	23
5	F43	D	552	62/62	0.99	0.03	4,7,9,12	0
6	TP7	A	553[A]	21/21	0.99	0.04	7,8,10,13	21
4	MG	D	551	1/1	0.99	0.16	24,24,24,24	0
7	COM	A	554	7/7	0.99	0.05	9,9,12,12	7
7	COM	D	554	7/7	0.99	0.06	9,10,12,13	0
5	F43	A	1	62/62	0.99	0.03	5,7,10,13	0
11	ZN	A	558	1/1	1.00	0.04	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.

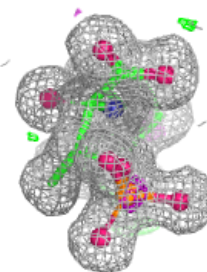
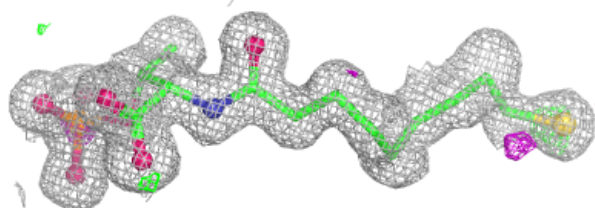
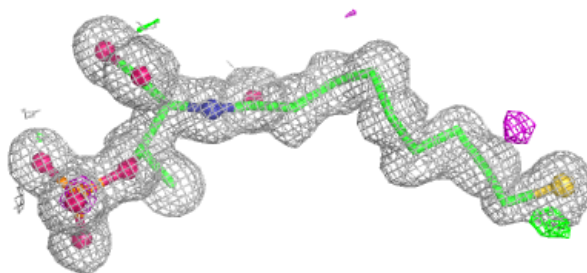
Electron density around XP9 D 555 (B):

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

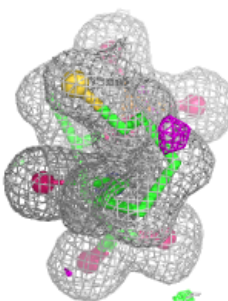
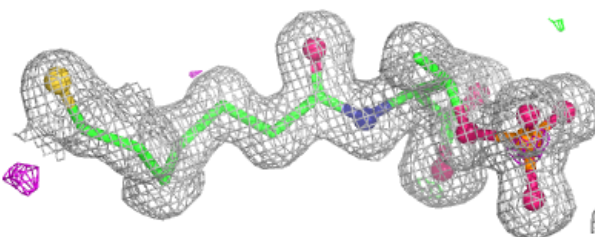
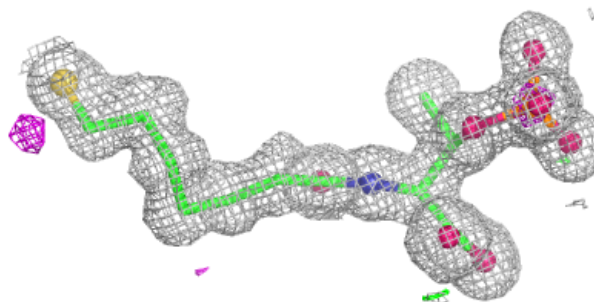


Electron density around XP9 D 555 (C):

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

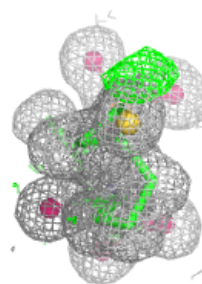
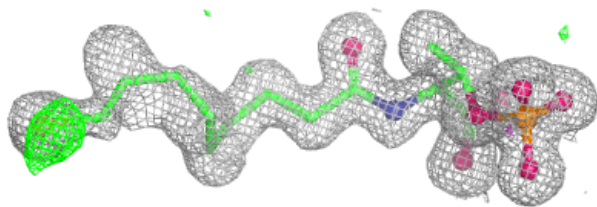
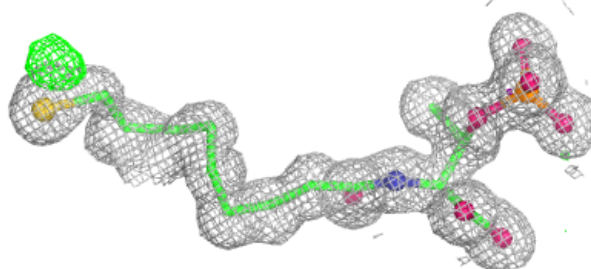
**Electron density around TP7 D 553 (A):**

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

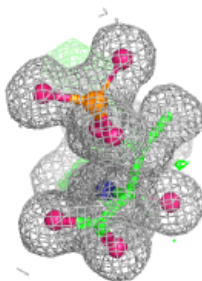
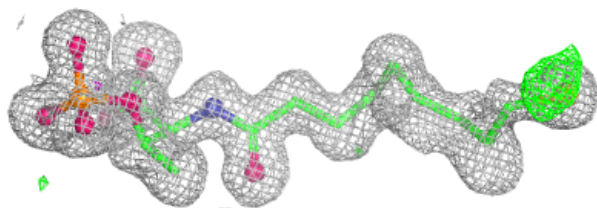
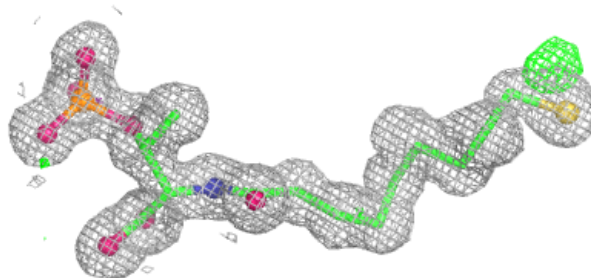


Electron density around XP9 A 555 (B):

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

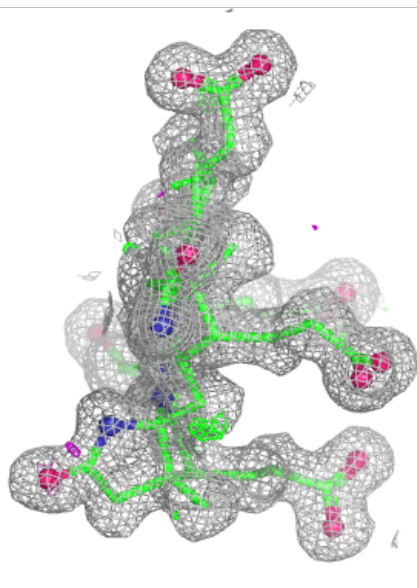
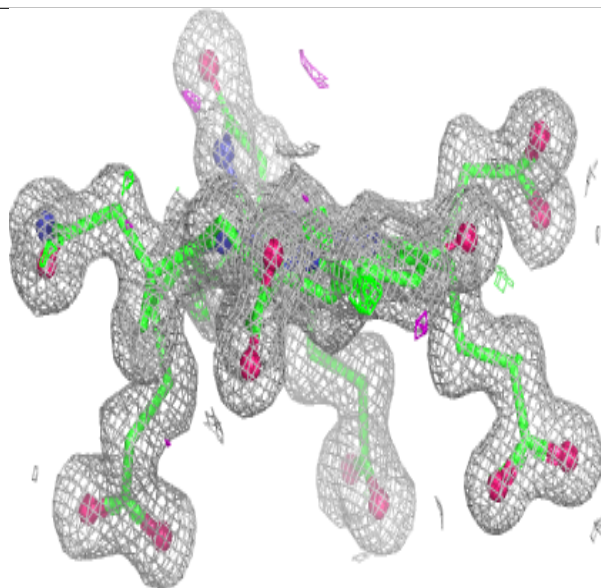
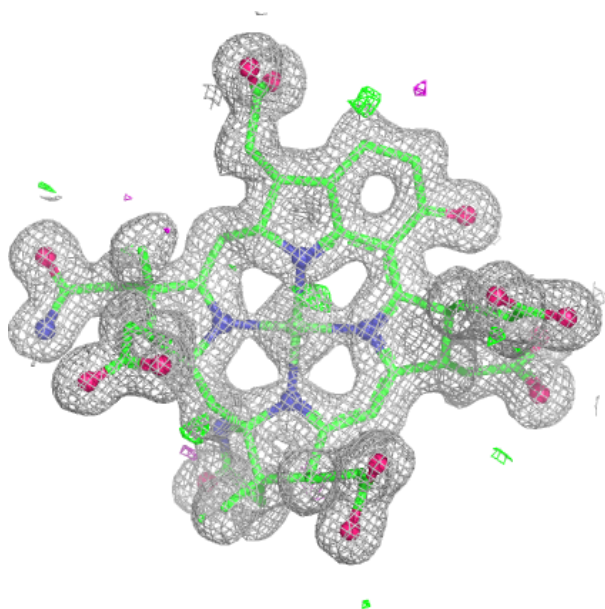
**Electron density around XP9 A 555 (C):**

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



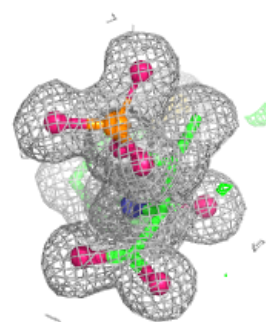
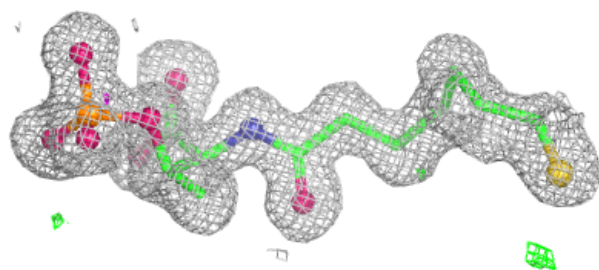
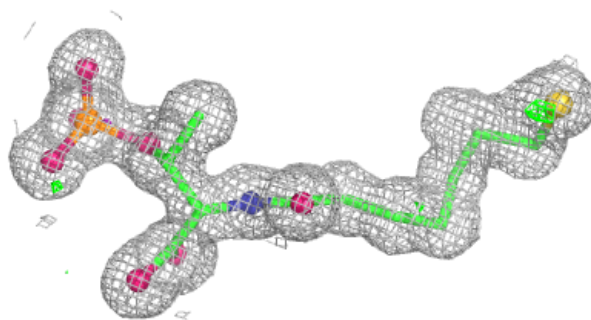
Electron density around F43 D 552:

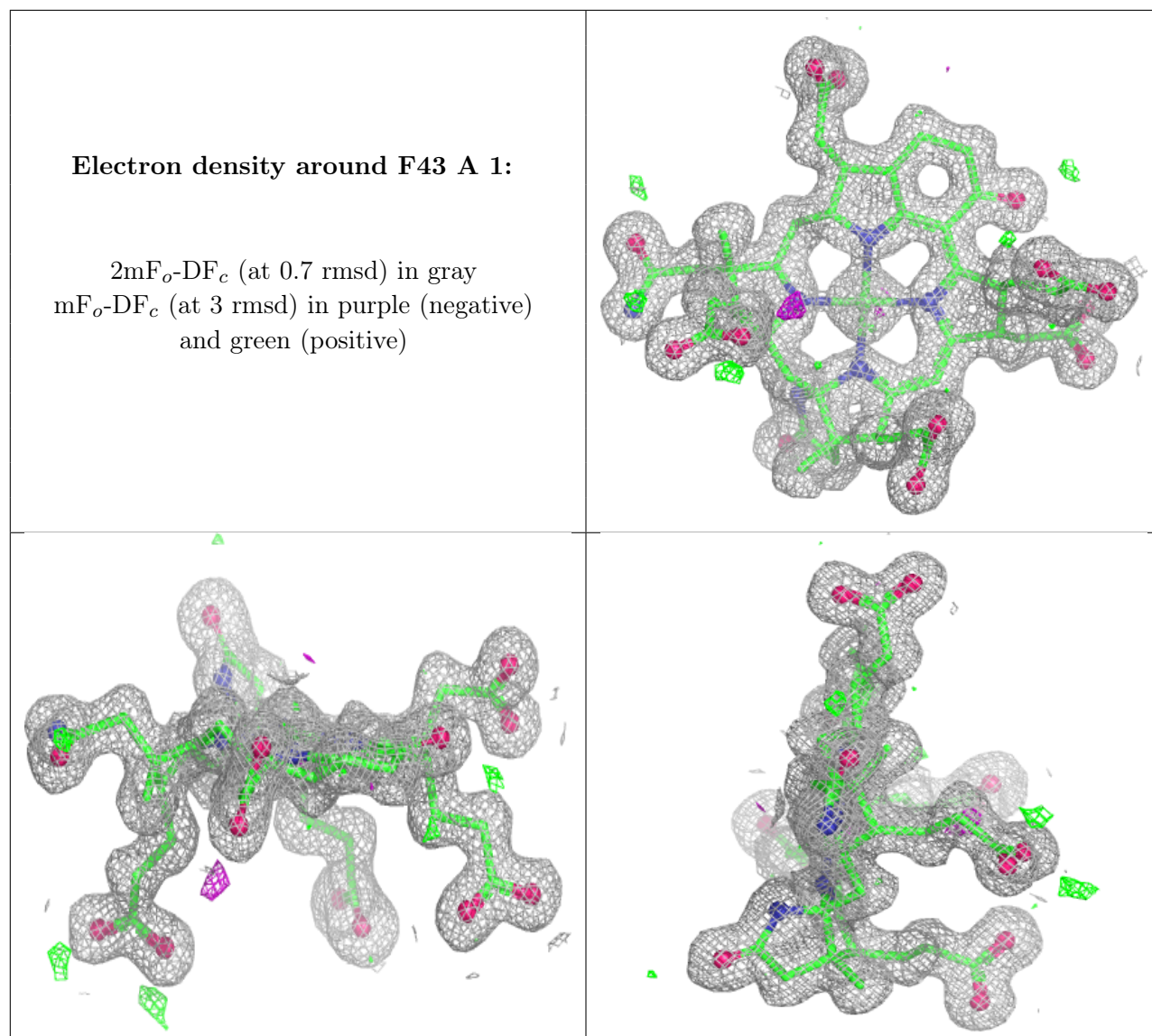
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TP7 A 553 (A):

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





6.5 Other polymers [i](#)

There are no such residues in this entry.