



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:51 PM EDT

PDB ID : 3M2R / pdb_00003m2r
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 : 1.30 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

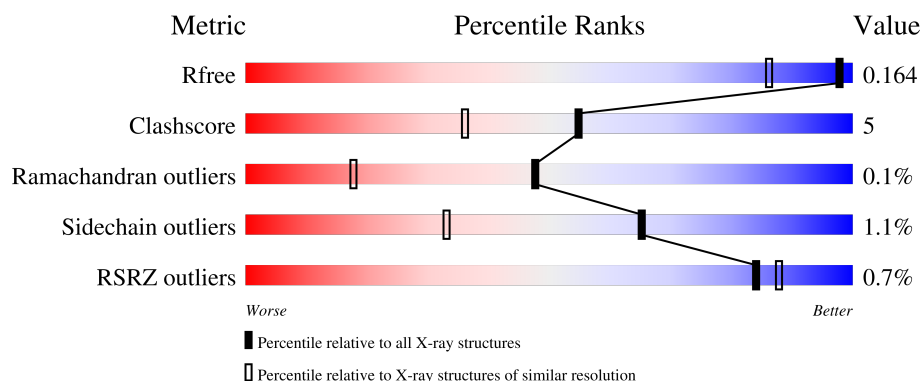
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	80% 18% .
1	D	549	2% 79% 19% .
2	B	442	79% 19% .
2	E	442	79% 21%
3	C	248	2% 73% 25% ..

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Mol	Chain	Length	Quality of chain
3	F	248	2% 73% 24% ..

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 22783 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	29	0
			4438	2809	731	878	20			
1	D	548	Total	C	N	O	S	0	30	0
			4426	2813	730	863	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	24	0
			3456	2205	559	670	22			
2	E	442	Total	C	N	O	S	0	31	0
			3509	2240	569	677	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	20	0
			2135	1320	375	426	14			
3	F	246	Total	C	N	O	S	0	22	0
			2121	1316	371	419	15			

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

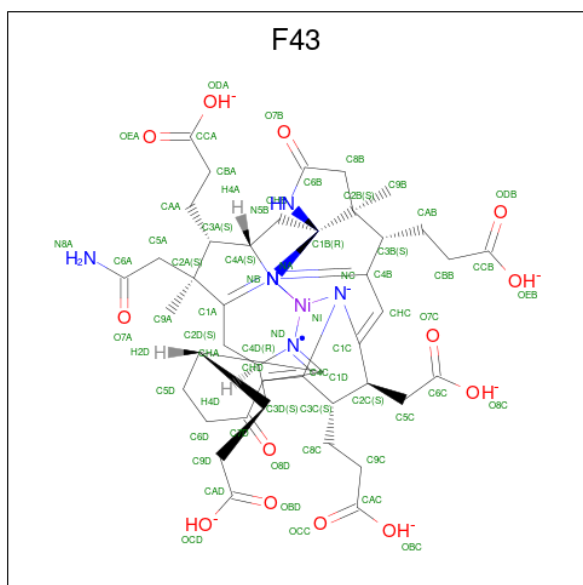
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	2
			3	3		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	2	Total	Mg	0	0
			2	2		

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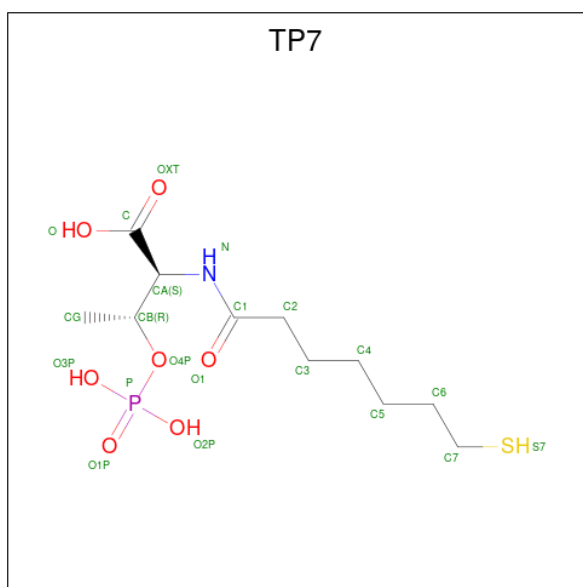
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is FACTOR 430 (CCD ID: F43) (formula: $\text{C}_{42}\text{H}_{51}\text{N}_6\text{NiO}_{13}$).



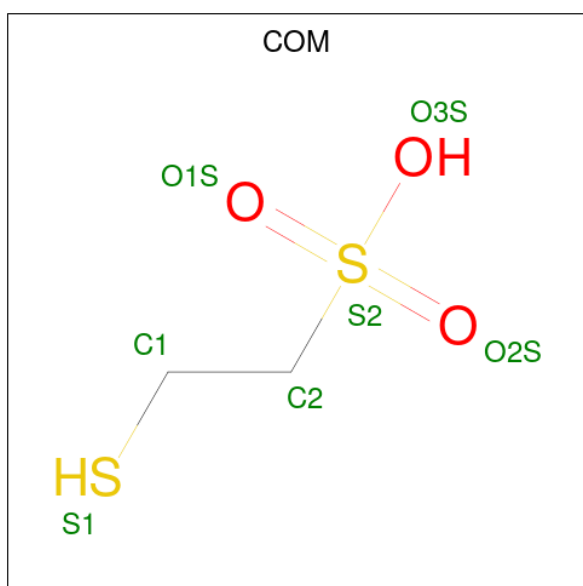
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
5	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

- Molecule 6 is Coenzyme B (CCD ID: TP7) (formula: $\text{C}_{11}\text{H}_{22}\text{NO}_7\text{PS}$).



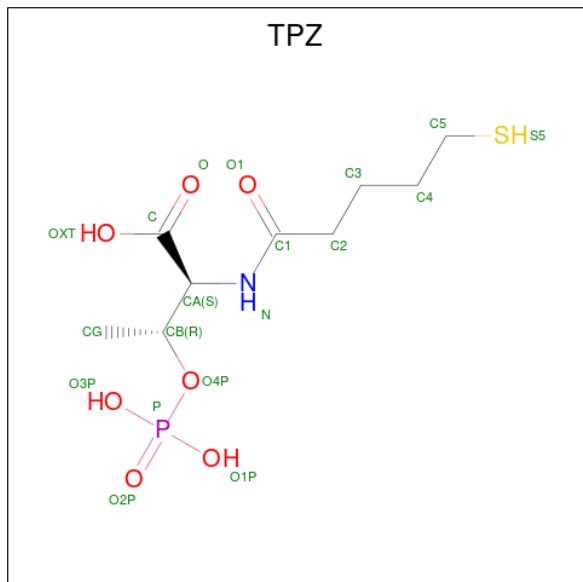
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

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



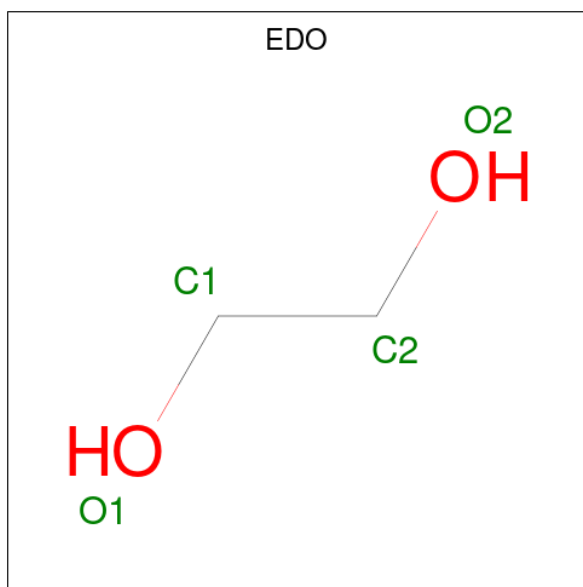
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is O-phosphono-N-(5-sulfanylpentanoyl)-L-threonine (CCD ID: TPZ) (formula: $C_9H_{18}NO_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			19	9	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	1
			19	9	1	7	1	1		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

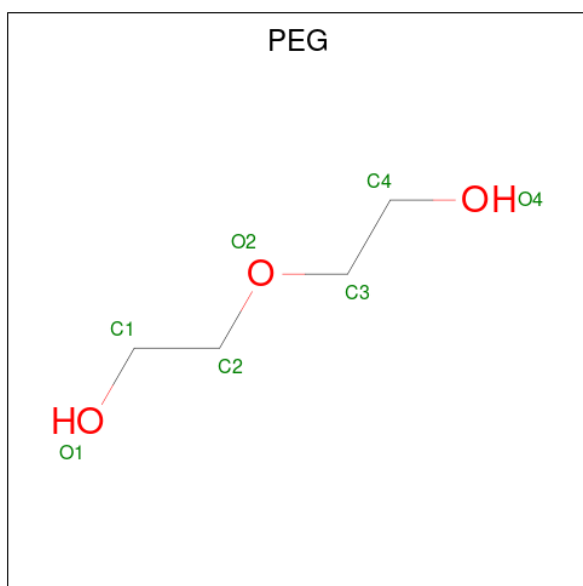


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

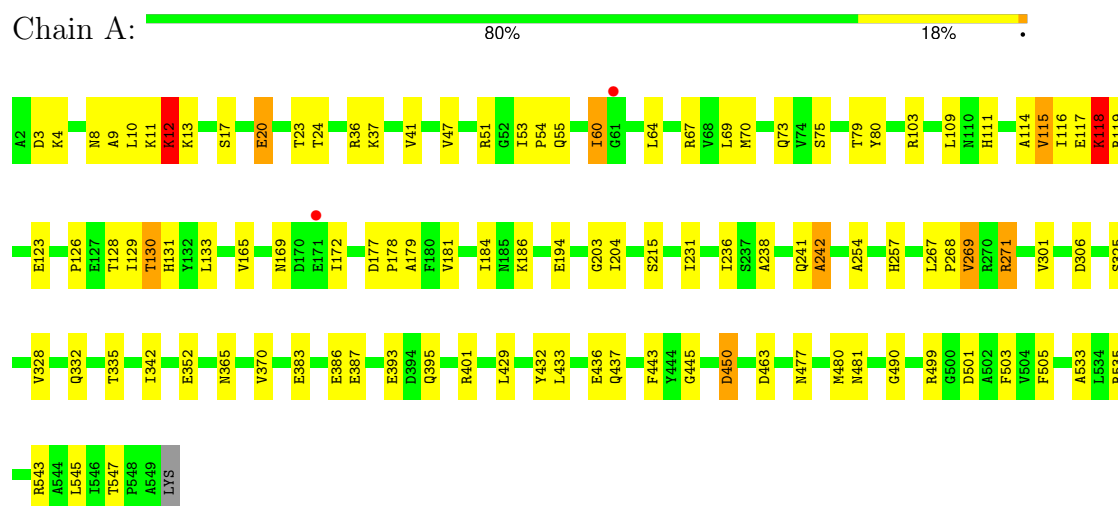
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	513	Total 520	O 520	0	18
12	B	451	Total 461	O 461	0	17
12	C	256	Total 259	O 259	0	5
12	D	520	Total 526	O 526	0	15
12	E	418	Total 423	O 423	0	16
12	F	250	Total 254	O 254	0	8

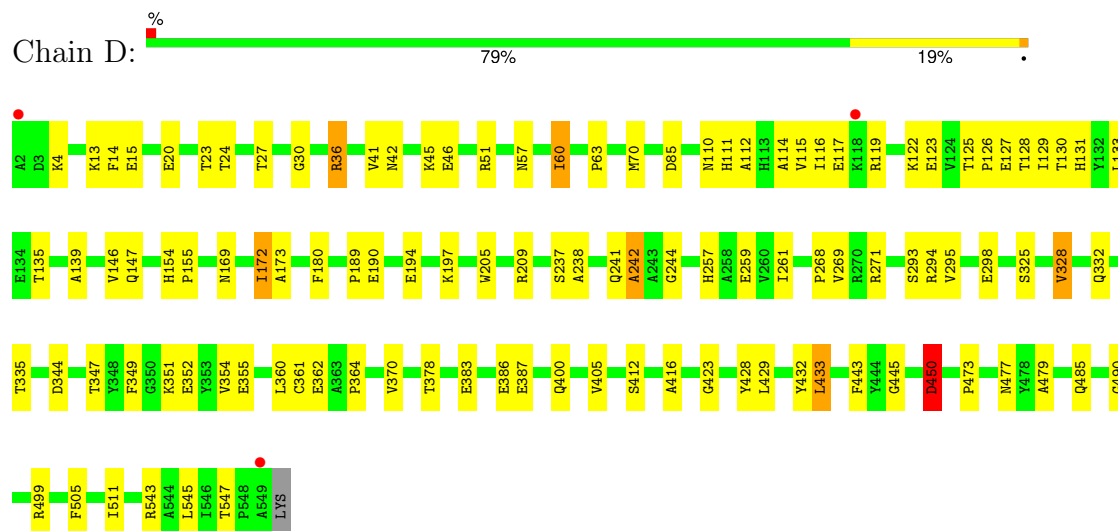
3 Residue-property plots

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

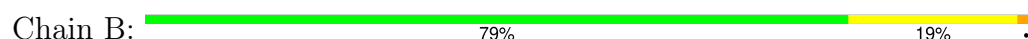
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

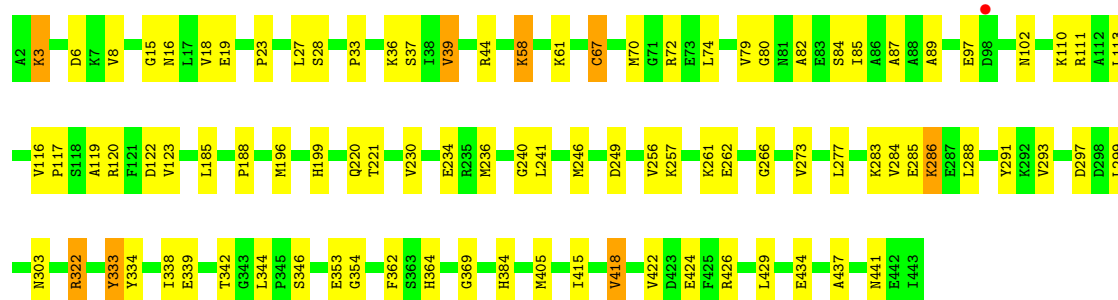


- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



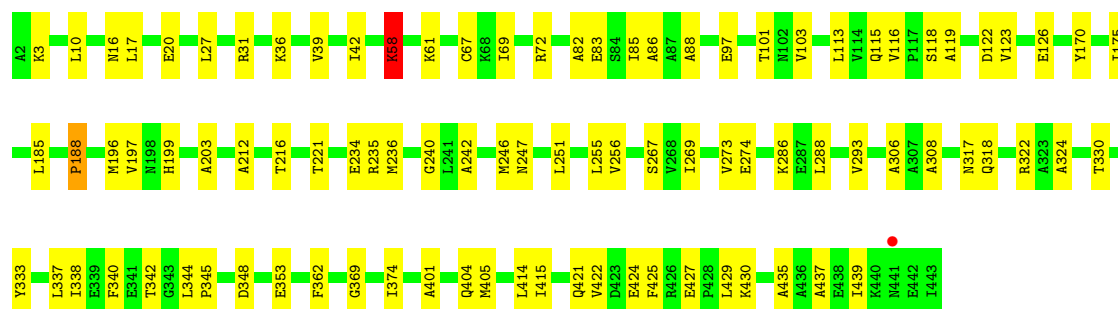
- Molecule 2: Methyl-coenzyme M reductase I subunit beta





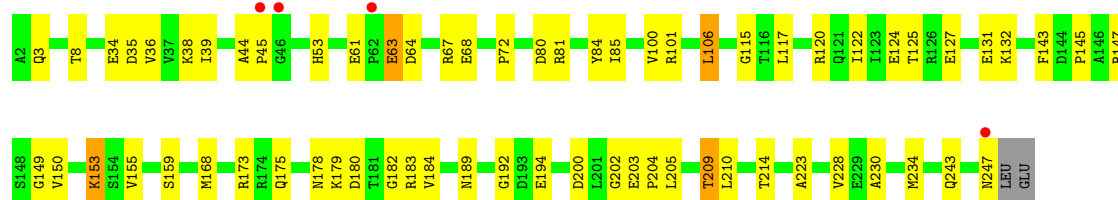
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E: 79% 21%



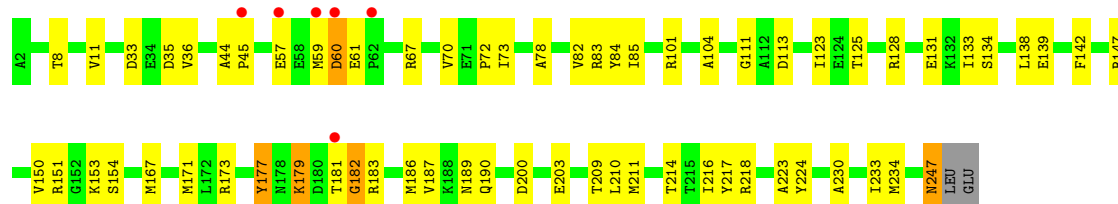
• Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C: 2% 73% 25%



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

Chain F: 2% 73% 24%



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)	20.49 – 1.30 20.49 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.49-1.30) 97.1 (20.49-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.143 , 0.166 0.142 , 0.164	Depositor DCC
R_{free} test set	27777 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	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 0.006 for -h,-l,-k 0.012 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22783	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 3.04% 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: TPZ, EDO, ZN, MHS, PEG, TP7, SMC, MGN, F43, AGM, COM, GL3, MG

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	1.80	56/4536 (1.2%)	1.53	33/6160 (0.5%)
1	D	1.85	70/4544 (1.5%)	1.54	30/6168 (0.5%)
2	B	1.84	52/3573 (1.5%)	1.50	14/4834 (0.3%)
2	E	1.82	48/3632 (1.3%)	1.47	20/4910 (0.4%)
3	C	2.01	44/2194 (2.0%)	1.59	14/2952 (0.5%)
3	F	2.00	38/2203 (1.7%)	1.71	20/2962 (0.7%)
All	All	1.87	308/20682 (1.5%)	1.54	131/27986 (0.5%)

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	3
1	D	1	1
2	B	0	2
2	E	0	2
All	All	2	8

All (308) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	VAL	CA-CB	11.63	1.71	1.54
1	A	450	ASP	CA-CB	-10.86	1.36	1.53
1	D	129	ILE	CA-CB	-10.28	1.42	1.54
1	D	269	VAL	CA-CB	10.18	1.67	1.54
1	D	450	ASP	CA-CB	-9.42	1.38	1.53
1	D	416	ALA	C-O	8.38	1.33	1.24
2	B	284	VAL	C-O	8.17	1.32	1.24
1	D	131	HIS	CA-C	8.17	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	85	ILE	N-CA	7.94	1.55	1.46
1	D	237	SER	C-O	7.84	1.33	1.24
3	C	155	VAL	CA-CB	7.68	1.64	1.54
2	B	437	ALA	CA-C	-7.66	1.43	1.52
2	B	286	LYS	N-CA	7.60	1.55	1.45
1	A	60	ILE	CA-CB	7.59	1.64	1.54
3	C	143	PHE	C-O	7.55	1.32	1.24
1	A	37	LYS	N-CA	-7.53	1.37	1.46
1	D	114	ALA	CA-CB	-7.47	1.41	1.53
3	C	204	PRO	N-CA	7.44	1.55	1.47
3	C	72	PRO	C-O	7.43	1.32	1.23
3	C	228	VAL	CA-CB	7.42	1.65	1.54
2	B	241	LEU	N-CA	-7.39	1.37	1.46
1	A	238	ALA	C-O	7.31	1.33	1.24
3	C	36	VAL	N-CA	7.26	1.55	1.46
3	F	217	TYR	CA-C	-7.26	1.43	1.52
1	D	146	VAL	CA-C	-7.25	1.45	1.52
1	A	60	ILE	CA-C	7.22	1.61	1.52
1	D	127	GLU	N-CA	-7.21	1.37	1.46
3	C	34	GLU	N-CA	-7.20	1.37	1.46
1	D	450	ASP	CA-C	-7.16	1.43	1.52
1	A	69	LEU	CA-C	-7.10	1.44	1.52
2	B	23	PRO	CA-C	7.08	1.61	1.52
3	F	189	ASN	CA-C	7.08	1.63	1.53
2	E	240	GLY	N-CA	7.02	1.54	1.45
2	B	85	ILE	CA-CB	-7.01	1.46	1.54
3	C	209	THR	N-CA	-7.00	1.37	1.46
3	F	70	VAL	CA-CB	6.99	1.62	1.53
1	A	11	LYS	N-CA	6.98	1.54	1.46
3	F	210	LEU	N-CA	6.98	1.54	1.46
3	C	36	VAL	CA-CB	-6.94	1.45	1.54
3	C	153	LYS	C-O	6.92	1.31	1.23
1	D	205	TRP	N-CA	6.90	1.54	1.46
3	F	73	ILE	CA-CB	6.86	1.60	1.54
2	B	28	SER	CA-C	-6.82	1.45	1.53
3	F	187	VAL	CA-CB	-6.82	1.47	1.54
2	B	273	VAL	CA-C	6.75	1.61	1.52
2	B	291	TYR	N-CA	6.72	1.53	1.46
1	D	112	ALA	N-CA	-6.71	1.38	1.46
1	D	543	ARG	CB-CG	6.68	1.72	1.52
1	D	20	GLU	C-O	6.63	1.31	1.23
1	D	173	ALA	N-CA	6.63	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	117	PRO	C-O	6.59	1.31	1.23
2	B	8	VAL	CA-CB	6.52	1.66	1.54
3	C	3	GLN	CA-CB	6.52	1.63	1.53
3	F	173	ARG	C-O	6.51	1.32	1.23
1	D	111	HIS	CA-C	-6.51	1.44	1.52
3	F	82	VAL	N-CA	6.51	1.54	1.46
1	A	73	GLN	N-CA	-6.51	1.38	1.46
3	F	134	SER	N-CA	-6.49	1.38	1.46
1	D	347	THR	CA-C	6.46	1.61	1.52
1	A	116	ILE	CA-CB	-6.44	1.46	1.54
1	D	114	ALA	N-CA	6.40	1.54	1.46
1	D	126	PRO	CA-C	-6.36	1.42	1.52
1	A	203	GLY	N-CA	6.34	1.53	1.45
1	D	354	VAL	CA-CB	6.33	1.62	1.54
1	D	110	ASN	CA-CB	-6.32	1.43	1.53
1	D	110	ASN	N-CA	6.32	1.53	1.46
1	A	64	LEU	C-O	6.31	1.31	1.23
2	B	19	GLU	CA-C	-6.27	1.45	1.52
3	F	60	ASP	CA-C	6.26	1.61	1.53
2	B	240	GLY	N-CA	6.22	1.53	1.45
2	E	85	ILE	CA-CB	-6.22	1.47	1.54
3	C	149	GLY	C-O	6.22	1.32	1.23
3	F	247	ASN	CG-OD1	6.21	1.35	1.23
3	C	106	LEU	C-O	-6.21	1.16	1.24
1	D	27	THR	CA-CB	6.20	1.63	1.53
2	B	354	GLY	N-CA	6.19	1.53	1.45
3	C	168	MET	N-CA	6.16	1.53	1.46
2	B	67	CYS	C-O	6.16	1.31	1.23
2	B	422	VAL	N-CA	-6.16	1.39	1.46
2	E	288	LEU	C-O	6.15	1.29	1.23
2	E	256	VAL	CA-C	6.14	1.60	1.52
3	F	190	GLN	N-CA	6.13	1.54	1.46
1	A	267	LEU	C-O	6.12	1.30	1.24
1	A	130	THR	CA-C	6.09	1.60	1.52
3	F	85	ILE	CA-C	6.09	1.60	1.52
1	D	349	PHE	CA-C	-6.08	1.45	1.52
2	E	269	ILE	CA-CB	-6.07	1.47	1.54
2	E	216	THR	CA-C	-6.03	1.45	1.52
1	D	405	VAL	C-O	6.02	1.30	1.24
2	E	286	LYS	CA-CB	6.00	1.63	1.53
3	C	223	ALA	N-CA	6.00	1.53	1.46
2	B	293	VAL	CA-CB	-5.99	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ALA	CA-CB	5.99	1.62	1.53
1	A	543	ARG	CB-CG	5.99	1.70	1.52
3	C	204	PRO	C-O	5.98	1.31	1.23
2	B	39	VAL	CA-C	-5.97	1.45	1.52
1	D	259	GLU	CG-CD	5.97	1.67	1.52
1	D	242	ALA	CA-CB	5.96	1.63	1.53
3	F	101	ARG	NE-CZ	5.96	1.39	1.33
2	B	84	SER	C-O	-5.95	1.17	1.24
2	E	267	SER	CA-C	-5.94	1.44	1.52
3	C	100	VAL	N-CA	5.94	1.53	1.46
2	B	338	ILE	C-O	5.91	1.31	1.24
3	F	154	SER	C-O	5.91	1.32	1.23
1	A	10	LEU	C-O	-5.90	1.17	1.24
3	C	200	ASP	CG-OD2	-5.89	1.14	1.25
3	C	85	ILE	C-O	5.89	1.29	1.24
3	F	139	GLU	CD-OE2	5.88	1.36	1.25
3	C	243[A]	GLN	CA-C	-5.86	1.45	1.52
3	C	243[B]	GLN	CA-C	-5.86	1.45	1.52
1	A	236	ILE	C-O	5.85	1.30	1.24
1	A	254	ALA	N-CA	5.85	1.53	1.46
1	D	133	LEU	CA-C	-5.83	1.45	1.52
1	D	238	ALA	C-O	5.82	1.31	1.24
2	B	16	ASN	N-CA	5.82	1.53	1.46
1	A	131	HIS	CA-C	5.82	1.60	1.52
1	A	342	ILE	CA-CB	-5.81	1.47	1.54
3	C	159	SER	C-O	-5.80	1.16	1.24
3	C	214	THR	N-CA	5.78	1.53	1.45
1	A	3	ASP	CA-C	5.76	1.59	1.52
2	B	6	ASP	CA-C	-5.76	1.45	1.52
3	C	223	ALA	CA-CB	-5.75	1.44	1.53
3	F	125	THR	CA-C	5.75	1.59	1.52
2	E	216	THR	CA-CB	5.74	1.62	1.53
2	E	251	LEU	C-O	-5.74	1.17	1.24
1	A	395	GLN	CA-C	-5.73	1.47	1.53
1	A	370	VAL	N-CA	5.73	1.53	1.46
2	E	404	GLN	CA-C	-5.72	1.45	1.52
2	E	427	GLU	CA-C	-5.72	1.45	1.52
1	D	378	THR	N-CA	5.71	1.53	1.46
3	F	216	ILE	CA-CB	5.71	1.61	1.54
1	D	511	ILE	CA-CB	5.70	1.61	1.54
1	A	365	ASN	CA-C	-5.68	1.46	1.53
1	D	433	LEU	CA-C	-5.68	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	212	ALA	C-O	5.68	1.30	1.24
1	A	545	LEU	C-O	5.67	1.31	1.24
3	C	173	ARG	N-CA	5.67	1.54	1.46
2	E	69	ILE	CA-CB	-5.67	1.47	1.53
3	F	33	ASP	CA-C	-5.66	1.45	1.52
3	C	175	GLN	C-N	5.66	1.40	1.33
2	E	82	ALA	CA-C	-5.66	1.45	1.52
1	D	351	LYS	CA-C	5.65	1.59	1.52
3	F	230	ALA	N-CA	5.65	1.53	1.46
1	A	501	ASP	N-CA	5.65	1.52	1.46
3	C	173	ARG	CA-C	-5.64	1.46	1.53
1	D	116	ILE	CA-C	5.64	1.59	1.52
2	B	89	ALA	N-CA	5.64	1.53	1.46
3	C	209	THR	CA-C	5.63	1.60	1.52
2	E	101	THR	C-O	5.63	1.30	1.23
2	E	439	ILE	CA-CB	5.62	1.61	1.54
3	F	128	ARG	NE-CZ	5.60	1.39	1.33
3	F	113	ASP	N-CA	5.59	1.54	1.46
1	A	306	ASP	N-CA	5.59	1.53	1.46
2	B	85	ILE	N-CA	5.56	1.53	1.46
2	E	306	ALA	CA-C	5.56	1.60	1.52
2	E	421	GLN	CA-C	-5.56	1.45	1.52
1	A	115	VAL	C-O	5.56	1.30	1.24
1	D	14	PHE	N-CA	5.56	1.52	1.45
1	D	4	LYS	N-CA	5.56	1.52	1.46
1	D	423	GLY	CA-C	5.55	1.58	1.51
1	D	135	THR	CA-C	5.55	1.59	1.52
3	F	209	THR	CA-C	5.54	1.59	1.52
3	F	223	ALA	CA-C	-5.53	1.45	1.52
1	A	23	THR	CA-CB	5.53	1.61	1.53
1	D	117	GLU	N-CA	5.53	1.53	1.46
2	B	249	ASP	N-CA	5.53	1.52	1.46
2	E	353	GLU	CG-CD	5.53	1.65	1.52
1	A	386	GLU	N-CA	5.52	1.53	1.46
2	B	102	ASN	CA-C	-5.52	1.45	1.52
1	A	23	THR	C-O	-5.52	1.18	1.23
1	D	123	GLU	CA-C	5.52	1.60	1.52
3	C	247	ASN	CG-ND2	5.51	1.44	1.33
2	E	348	ASP	CA-CB	5.51	1.61	1.53
1	A	436	GLU	C-O	5.51	1.31	1.24
1	A	119	ARG	CB-CG	-5.50	1.35	1.52
2	E	435	ALA	CA-CB	5.49	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	GLN	C-O	5.48	1.30	1.23
2	B	266	GLY	C-O	5.47	1.30	1.23
3	C	35	ASP	CA-C	5.47	1.60	1.52
1	A	181	VAL	CA-CB	5.47	1.61	1.54
2	B	87	ALA	CA-CB	5.47	1.61	1.53
3	C	81	ARG	CD-NE	5.46	1.53	1.46
2	E	308	ALA	CA-C	-5.46	1.45	1.52
1	D	490	GLY	C-O	5.46	1.30	1.23
1	D	244	GLY	C-O	5.45	1.31	1.23
2	B	80	GLY	N-CA	5.44	1.52	1.45
2	E	330	THR	N-CA	5.44	1.52	1.46
2	B	110	LYS	N-CA	5.43	1.53	1.46
3	C	189	ASN	CA-C	5.41	1.60	1.53
1	D	190	GLU	CA-CB	5.41	1.61	1.53
1	A	53	ILE	N-CA	5.41	1.53	1.46
3	F	83	ARG	CA-C	5.39	1.60	1.52
1	D	63	PRO	CA-CB	5.39	1.61	1.53
1	D	294	ARG	CZ-NH1	5.38	1.40	1.32
2	E	115	GLN	C-O	5.38	1.30	1.24
1	D	197	LYS	CD-CE	-5.38	1.36	1.52
2	B	285	GLU	N-CA	-5.37	1.39	1.46
2	B	120	ARG	CZ-NH1	5.37	1.40	1.32
1	D	70	MET	C-O	5.37	1.30	1.23
2	E	31	ARG	CA-C	-5.37	1.45	1.52
1	A	60	ILE	C-N	-5.37	1.24	1.33
1	D	189	PRO	N-CA	5.36	1.53	1.47
1	D	362	GLU	N-CA	5.36	1.53	1.46
3	C	155	VAL	C-O	5.36	1.30	1.24
1	D	386	GLU	CD-OE1	5.36	1.35	1.25
3	F	36	VAL	CA-CB	-5.33	1.48	1.54
2	E	337	LEU	CA-C	-5.33	1.45	1.52
1	A	54	PRO	CA-CB	5.32	1.60	1.53
3	C	122	ILE	CA-C	-5.31	1.46	1.52
1	D	130	THR	CB-OG1	-5.31	1.35	1.43
2	B	286	LYS	CA-CB	5.30	1.63	1.53
1	A	47	VAL	CA-C	-5.29	1.46	1.52
2	B	418	VAL	C-O	5.28	1.29	1.23
1	A	111	HIS	CA-C	-5.28	1.46	1.52
1	D	125	THR	CA-CB	5.28	1.60	1.53
1	D	485	GLN	N-CA	5.28	1.52	1.46
2	E	86	ALA	CA-C	-5.27	1.46	1.52
3	C	53	HIS	CA-CB	5.27	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	33	PRO	CA-CB	5.26	1.61	1.53
2	E	247	ASN	C-O	5.26	1.30	1.23
2	E	422	VAL	N-CA	-5.26	1.40	1.46
1	D	261	ILE	CG1-CD1	-5.25	1.31	1.51
1	D	543	ARG	CG-CD	-5.25	1.36	1.52
3	C	230	ALA	CA-CB	-5.25	1.45	1.53
1	A	79	THR	C-O	5.24	1.30	1.24
1	A	118	LYS	C-O	5.24	1.30	1.23
1	A	503	PHE	N-CA	5.24	1.52	1.45
2	B	70	MET	N-CA	5.23	1.52	1.46
2	B	338	ILE	CA-C	-5.23	1.45	1.52
3	C	53	HIS	N-CA	-5.23	1.41	1.46
3	F	138	LEU	CA-C	5.23	1.59	1.52
2	B	79	VAL	CA-CB	-5.22	1.47	1.54
3	F	133	ILE	C-O	5.22	1.30	1.24
1	A	20	GLU	CA-C	-5.22	1.46	1.52
1	A	301	VAL	N-CA	-5.22	1.40	1.46
3	C	8	THR	N-CA	5.22	1.51	1.46
2	E	414	LEU	CA-C	-5.21	1.46	1.52
1	D	360	LEU	N-CA	5.21	1.52	1.46
1	A	4	LYS	N-CA	5.20	1.52	1.45
2	E	203	ALA	C-O	5.19	1.30	1.24
2	E	16	ASN	CA-C	-5.19	1.46	1.52
3	F	224	TYR	CA-C	5.18	1.59	1.52
2	E	340	PHE	C-O	5.18	1.30	1.24
1	D	344	ASP	N-CA	5.18	1.52	1.46
2	B	384	HIS	ND1-CE1	5.17	1.37	1.32
1	D	60[A]	ILE	CA-CB	5.17	1.61	1.54
1	D	60[B]	ILE	CA-CB	5.17	1.61	1.54
3	F	147	ARG	CD-NE	5.17	1.53	1.46
2	B	39	VAL	C-O	5.17	1.29	1.24
2	E	242	ALA	N-CA	5.17	1.52	1.46
2	E	401	ALA	C-O	5.16	1.30	1.24
3	C	3	GLN	CB-CG	-5.16	1.36	1.52
1	D	30	GLY	N-CA	5.16	1.54	1.45
2	E	324	ALA	C-N	-5.16	1.27	1.33
2	E	430	LYS	N-CA	-5.16	1.40	1.46
2	B	240	GLY	CA-C	-5.15	1.46	1.52
2	B	334	TYR	CA-C	-5.15	1.46	1.52
2	E	235	ARG	CZ-NH2	5.15	1.40	1.33
1	A	75	SER	CA-C	-5.14	1.46	1.52
3	C	63	GLU	CA-C	5.14	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	THR	N-CA	-5.14	1.38	1.46
2	E	58	LYS	CB-CG	-5.14	1.37	1.52
2	B	256	VAL	CA-CB	-5.13	1.48	1.54
3	F	247	ASN	CA-CB	5.13	1.63	1.53
2	E	10	LEU	C-O	5.12	1.30	1.24
3	C	80	ASP	C-O	5.11	1.30	1.23
1	D	370	VAL	N-CA	5.11	1.52	1.46
2	E	338	ILE	C-O	5.11	1.30	1.24
1	D	41	VAL	CA-C	5.10	1.59	1.52
3	F	217	TYR	C-O	5.10	1.30	1.24
2	E	175	ILE	C-O	5.09	1.29	1.23
2	B	437	ALA	C-O	5.09	1.30	1.24
1	A	437	GLN	N-CA	5.08	1.52	1.46
2	B	441	ASN	CA-C	-5.08	1.45	1.52
1	A	393	GLU	C-N	-5.08	1.27	1.33
3	F	72	PRO	C-O	5.08	1.29	1.23
1	A	12[A]	LYS	C-O	5.08	1.30	1.24
1	A	12[B]	LYS	C-O	5.08	1.30	1.24
2	B	364	HIS	N-CA	5.07	1.51	1.46
2	B	220	GLN	C-O	5.07	1.30	1.24
2	B	277	LEU	C-O	5.07	1.30	1.24
1	D	364	PRO	N-CA	-5.07	1.41	1.47
3	C	132	LYS	CA-CB	-5.07	1.45	1.53
2	E	404	GLN	C-O	5.07	1.30	1.24
3	F	8	THR	CA-C	-5.07	1.46	1.52
3	C	210	LEU	N-CA	5.06	1.52	1.46
3	F	104	ALA	CA-CB	-5.05	1.45	1.53
1	A	165	VAL	N-CA	-5.05	1.40	1.46
1	D	112	ALA	CA-C	5.05	1.59	1.52
1	A	133	LEU	C-O	5.05	1.30	1.24
1	A	242	ALA	C-N	-5.05	1.27	1.33
1	A	80	TYR	N-CA	-5.04	1.40	1.46
1	A	130	THR	N-CA	-5.04	1.40	1.46
2	B	82	ALA	CA-CB	-5.04	1.45	1.53
1	D	209	ARG	CB-CG	5.04	1.67	1.52
1	D	412	SER	CA-C	-5.04	1.46	1.52
3	F	154	SER	CA-C	-5.04	1.47	1.53
2	B	111	ARG	CD-NE	5.03	1.53	1.46
1	D	15	GLU	N-CA	5.03	1.52	1.46
3	F	218	ARG	CZ-NH1	5.03	1.39	1.32
3	C	38	LYS	CA-CB	5.03	1.61	1.53
2	B	322	ARG	CZ-NH1	5.03	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	170	TYR	CA-C	-5.02	1.48	1.53
1	D	27	THR	C-N	5.02	1.40	1.33
2	E	274[A]	GLU	C-O	5.02	1.30	1.24
2	E	274[B]	GLU	C-O	5.02	1.30	1.24
2	B	426	ARG	CZ-NH2	5.01	1.40	1.33
3	F	142	PHE	C-O	5.01	1.30	1.24

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	LEU	O-C-N	9.32	132.00	122.12
1	A	13	LYS	N-CA-C	8.26	121.85	111.69
2	B	44	ARG	NE-CZ-NH1	8.08	129.58	121.50
1	A	450	ASP	CB-CA-C	7.99	124.05	110.79
3	F	182[A]	GLY	N-CA-C	-7.79	103.09	115.08
3	F	182[B]	GLY	N-CA-C	-7.79	103.09	115.08
2	B	196	MET	CG-SD-CE	-7.76	83.83	100.90
1	D	116	ILE	O-C-N	7.67	129.43	121.91
1	A	13	LYS	CA-C-O	7.56	128.63	120.24
2	B	15	GLY	O-C-N	7.25	131.31	122.32
1	A	401	ARG	NE-CZ-NH2	7.13	125.62	119.20
2	B	18	VAL	N-CA-C	-7.03	105.51	111.56
1	D	450	ASP	N-CA-CB	6.96	120.36	110.12
3	F	125	THR	O-C-N	6.93	130.41	122.99
2	E	97	GLU	CA-C-N	-6.93	112.26	122.86
2	E	97	GLU	C-N-CA	-6.93	112.26	122.86
1	D	450	ASP	CB-CA-C	6.93	122.29	110.79
1	A	535	ARG	NE-CZ-NH2	6.91	125.42	119.20
2	B	434	GLU	O-C-N	-6.86	114.33	122.15
1	A	238	ALA	CA-C-O	-6.85	111.71	119.79
3	C	175	GLN	CA-C-O	6.74	127.51	120.30
1	A	450	ASP	N-CA-CB	6.74	120.02	110.12
2	E	256	VAL	O-C-N	6.65	128.68	121.83
3	F	11	VAL	O-C-N	-6.53	115.41	121.94
3	F	214	THR	CA-C-O	6.48	128.92	121.47
2	B	273	VAL	O-C-N	6.42	128.10	121.87
1	D	111	HIS	O-C-N	-6.42	114.83	122.15
1	A	129	ILE	N-CA-C	-6.36	104.55	110.53
2	B	353	GLU	CG-CD-OE2	-6.32	103.86	118.40
1	D	477	ASN	CB-CG-ND2	6.27	125.81	116.40
2	E	103	VAL	CA-C-O	-6.26	114.17	120.31
2	E	353	GLU	OE1-CD-OE2	6.20	137.77	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	131	HIS	O-C-N	6.17	128.66	122.12
3	C	147	ARG	NE-CZ-NH1	6.15	127.65	121.50
2	E	437	ALA	N-CA-C	-6.14	104.67	111.36
2	B	286	LYS	N-CA-C	-6.13	99.36	108.99
2	E	269	ILE	O-C-N	6.11	128.05	121.94
1	D	126	PRO	O-C-N	-6.07	114.94	122.23
2	E	293	VAL	O-C-N	-6.06	115.54	122.94
1	D	293	SER	CA-C-O	-6.04	113.43	120.20
1	A	70	MET	CB-CA-C	-6.04	100.05	109.11
3	C	153	LYS	CG-CD-CE	-6.01	97.48	111.30
3	C	115	GLY	O-C-N	-5.99	118.70	123.49
3	F	167	MET	O-C-N	5.96	130.07	123.16
2	E	273	VAL	O-C-N	5.95	127.64	121.87
1	D	139	ALA	CA-C-O	-5.91	113.68	120.24
3	F	83	ARG	O-C-N	5.91	130.89	122.74
1	A	477	ASN	CA-CB-CG	5.90	118.50	112.60
3	F	83	ARG	CA-C-O	-5.88	114.67	121.49
3	F	78	ALA	N-CA-C	5.86	120.16	112.89
1	D	547	THR	O-C-N	5.86	126.30	121.32
1	D	4	LYS	CA-CB-CG	5.84	125.79	114.10
1	A	41	VAL	O-C-N	5.79	127.58	121.91
1	A	450	ASP	CA-CB-CG	5.76	118.36	112.60
2	B	74	LEU	CA-C-N	-5.75	114.63	123.14
2	B	74	LEU	C-N-CA	-5.75	114.63	123.14
1	D	119	ARG	CG-CD-NE	-5.74	99.36	112.00
1	D	351	LYS	N-CA-C	-5.74	104.94	111.14
1	D	416	ALA	O-C-N	-5.72	115.91	122.09
3	C	101	ARG	NH1-CZ-NH2	5.69	126.70	119.30
1	A	116	ILE	O-C-N	5.67	127.47	121.91
3	F	151	ARG	CG-CD-NE	-5.67	99.52	112.00
1	A	128	THR	N-CA-C	-5.67	105.24	111.82
3	F	123	ILE	O-C-N	5.66	129.15	123.10
1	A	117	GLU	CB-CG-CD	5.65	122.21	112.60
1	A	535	ARG	NE-CZ-NH1	-5.64	115.86	121.50
2	E	308	ALA	O-C-N	-5.64	116.14	122.12
3	C	39	ILE	O-C-N	5.64	127.34	121.87
3	F	177	TYR	O-C-N	-5.63	116.37	123.01
1	A	184	ILE	O-C-N	5.62	127.32	121.87
1	A	13	LYS	CB-CA-C	-5.61	100.44	110.70
3	C	131	GLU	O-C-N	5.60	128.05	122.12
3	F	133	ILE	O-C-N	-5.58	116.46	121.87
1	A	547	THR	CA-C-N	-5.57	114.52	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	THR	C-N-CA	-5.57	114.52	120.03
2	E	88	ALA	O-C-N	5.56	128.49	122.15
1	D	405	VAL	N-CA-C	-5.55	105.32	110.53
1	D	295[A]	VAL	O-C-N	-5.51	116.35	121.97
1	D	295[B]	VAL	O-C-N	-5.51	116.35	121.97
1	D	499	ARG	NH1-CZ-NH2	5.50	126.45	119.30
1	A	103	ARG	NE-CZ-NH2	-5.49	114.25	119.20
3	F	147	ARG	NE-CZ-NH1	5.49	126.99	121.50
3	F	131	GLU	CA-C-O	-5.49	113.66	119.97
1	D	172[A]	ILE	O-C-N	5.47	127.46	121.83
1	D	172[B]	ILE	O-C-N	5.47	127.46	121.83
3	F	85	ILE	O-C-N	5.44	129.09	123.05
2	E	188	PRO	O-C-N	-5.44	116.45	123.03
2	E	306	ALA	O-C-N	5.42	127.87	122.12
1	A	481	ASN	CA-C-O	5.42	126.45	120.71
1	A	70	MET	N-CA-C	5.39	118.11	110.24
2	E	126	GLU	CB-CA-C	5.38	121.12	110.42
1	D	135	THR	O-C-N	5.36	127.88	122.09
3	C	125	THR	CA-C-O	-5.36	115.58	121.31
2	E	337	LEU	CA-C-O	-5.36	114.87	120.55
1	D	328	VAL	O-C-N	5.33	127.12	121.89
2	E	185	LEU	CB-CG-CD1	5.32	126.65	110.70
1	A	231	ILE	N-CA-C	-5.26	105.37	110.42
1	A	490	GLY	O-C-N	5.25	127.23	122.19
1	A	543	ARG	CA-CB-CG	5.24	124.58	114.10
2	B	44	ARG	NE-CZ-NH2	-5.23	114.49	119.20
3	C	192	GLY	O-C-N	5.22	128.66	122.50
1	A	533	ALA	O-C-N	5.21	128.68	122.27
3	F	101	ARG	NH1-CZ-NH2	5.19	126.05	119.30
2	B	334	TYR	O-C-N	-5.19	116.62	122.12
1	A	67	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	D	490	GLY	CA-C-O	-5.17	115.42	120.75
1	D	128	THR	CA-C-O	-5.14	114.06	119.97
3	C	127	GLU	CA-C-N	-5.11	112.54	120.31
3	C	127	GLU	C-N-CA	-5.11	112.54	120.31
1	A	36	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	125	THR	CB-CA-C	-5.10	103.38	110.37
1	A	241	GLN	O-C-N	5.10	128.60	122.79
3	F	171	MET	O-C-N	5.09	128.00	122.20
2	E	255	LEU	N-CA-C	5.09	116.83	111.28
2	E	318	GLN	OE1-CD-NE2	5.09	127.69	122.60
2	B	230	VAL	CA-C-O	5.09	126.52	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	116	VAL	N-CA-CB	-5.07	104.77	109.99
1	D	190	GLU	N-CA-C	5.07	117.19	111.11
2	B	116	VAL	N-CA-CB	-5.07	104.12	111.21
1	D	180	PHE	O-C-N	-5.07	116.01	122.34
1	D	361	CYS	O-C-N	5.07	128.33	122.00
1	D	13	LYS	CB-CA-C	-5.06	102.25	110.85
1	D	123	GLU	CA-C-O	-5.06	115.65	121.47
3	F	35	ASP	CA-C-O	-5.05	114.16	119.97
3	C	101	ARG	NE-CZ-NH2	-5.04	114.66	119.20
3	C	131	GLU	CA-C-O	-5.04	115.20	120.55
3	F	233	ILE	O-C-N	5.04	127.03	121.83
1	A	8	ASN	O-C-N	-5.03	116.79	122.12
2	E	429	LEU	N-CA-C	-5.02	105.81	111.28
1	A	215	SER	N-CA-CB	-5.00	102.77	110.12
3	C	127	GLU	N-CA-C	5.00	117.11	111.11

All (2) chirality outliers are listed below:

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

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	MET	Peptide
1	A	499	ARG	Sidechain
1	A	51	ARG	Sidechain
2	B	333	TYR	Sidechain
2	B	72	ARG	Sidechain
1	D	51	ARG	Sidechain
2	E	333	TYR	Sidechain
2	E	72	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4438	0	4237	42	0
1	D	4426	0	4282	36	0
2	B	3456	0	3501	36	0
2	E	3509	0	3569	38	0
3	C	2135	0	2060	32	0
3	F	2121	0	2081	38	0
4	A	3	0	0	0	0
4	B	1	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	1	0
6	D	21	0	19	1	0
7	A	7	0	4	0	0
7	D	7	0	5	0	0
8	A	19	0	15	0	0
8	D	19	0	15	0	0
9	A	4	0	6	0	0
9	C	4	0	6	0	0
9	D	4	0	6	0	0
9	F	8	0	12	1	0
10	A	1	0	0	0	0
11	C	7	0	10	0	0
12	A	520	0	0	14	0
12	B	461	0	0	5	0
12	C	259	0	0	9	0
12	D	526	0	0	8	0
12	E	423	0	0	13	0
12	F	254	0	0	5	0
All	All	22783	0	19933	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:181[A]:THR:HB	3:F:183[A]:ARG:CD	1.70	1.20
1:A:429:LEU:HD12	3:C:234[B]:MET:HE1	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:CB	3:C:234[B]:MET:HE3	1.82	1.09
2:B:27:LEU:HD22	2:B:246[B]:MET:HE1	1.38	1.05
1:A:432:TYR:HB2	3:C:234[B]:MET:HE3	1.09	1.05
3:F:181[A]:THR:HB	3:F:183[A]:ARG:CG	1.85	1.05
3:F:181[A]:THR:CB	3:F:183[A]:ARG:HG3	1.92	0.99
2:B:27:LEU:CD2	2:B:246[B]:MET:HE1	1.93	0.98
1:A:429:LEU:CD1	3:C:234[B]:MET:HE1	1.93	0.97
1:D:24[A]:THR:HG23	12:F:1497:HOH:O	1.65	0.96
1:A:24[A]:THR:HG23	12:C:3803:HOH:O	1.64	0.96
1:A:352[A]:GLU:HG2	12:A:4100:HOH:O	1.65	0.94
1:A:433:LEU:HD23	3:C:234[B]:MET:SD	2.08	0.94
1:A:432:TYR:HB2	3:C:234[B]:MET:CE	1.98	0.93
2:B:61:LYS:HE3	12:B:2541:HOH:O	1.69	0.93
3:F:181[A]:THR:HB	3:F:183[A]:ARG:HG3	1.46	0.92
3:F:181[A]:THR:C	3:F:183[A]:ARG:HG3	1.95	0.92
3:C:124:GLU:HG3	12:C:4090:HOH:O	1.70	0.90
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:HB2	1.69	0.90
1:D:241[B]:GLN:HE21	1:D:241[B]:GLN:H	1.16	0.89
1:A:433:LEU:CD2	3:C:234[B]:MET:SD	2.62	0.88
3:F:181[A]:THR:HB	3:F:183[A]:ARG:HD3	1.56	0.87
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD12	1.91	0.86
3:F:181[A]:THR:CB	3:F:183[A]:ARG:CG	2.50	0.85
1:D:432:TYR:CB	3:F:234[B]:MET:HE3	2.08	0.82
3:F:181[A]:THR:CB	3:F:183[A]:ARG:CD	2.57	0.82
2:B:27:LEU:HD22	2:B:246[B]:MET:CE	2.10	0.80
1:D:46[B]:GLU:HG3	12:D:695:HOH:O	1.81	0.79
1:D:433:LEU:HD23	3:F:234[B]:MET:SD	2.22	0.79
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.12	0.79
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.65	0.79
2:E:61[A]:LYS:HE3	12:E:2470:HOH:O	1.83	0.79
1:D:432:TYR:HB2	3:F:234[B]:MET:HE3	1.64	0.78
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	1.66	0.77
1:D:429:LEU:HD12	3:F:234[B]:MET:HE1	1.67	0.76
1:D:194[B]:GLU:HG2	12:D:3701:HOH:O	1.86	0.76
12:A:3768:HOH:O	1:D:545:LEU:HD11	1.86	0.75
3:F:181[A]:THR:CB	3:F:183[A]:ARG:HD3	2.17	0.74
1:D:433:LEU:CD2	3:F:234[B]:MET:SD	2.75	0.74
1:A:178[A]:PRO:HD3	12:A:1631:HOH:O	1.88	0.74
2:B:261[A]:LYS:HG3	2:B:262:GLU:HG3	1.70	0.73
2:E:58:LYS:HE3	12:E:3968:HOH:O	1.85	0.73
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:CB	2.38	0.71
1:D:268:PRO:HB3	12:E:1668:HOH:O	1.92	0.70
1:A:130:THR:CG2	12:A:3696[B]:HOH:O	2.40	0.70
2:B:37[B]:SER:HB3	2:B:424[B]:GLU:OE1	1.91	0.70
1:A:268:PRO:HG3	12:A:4030:HOH:O	1.91	0.69
1:A:194[B]:GLU:HG2	12:A:2095:HOH:O	1.92	0.69
2:E:118[B]:SER:HB3	12:E:2658:HOH:O	1.93	0.68
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.22	0.68
3:F:200[A]:ASP:HB2	12:F:1920:HOH:O	1.94	0.67
1:D:241[B]:GLN:H	1:D:241[B]:GLN:NE2	1.92	0.66
1:D:42[A]:ASN:ND2	12:D:1802:HOH:O	2.27	0.66
1:A:12[B]:LYS:HG2	12:A:1449:HOH:O	1.95	0.65
2:E:83[A]:GLU:CG	12:E:3720:HOH:O	2.45	0.65
1:A:114:ALA:O	1:A:118:LYS:HD3	1.97	0.65
1:D:432:TYR:HB3	3:F:234[B]:MET:HE3	1.77	0.65
2:B:246[A]:MET:HE3	2:B:429:LEU:HD12	1.77	0.65
1:A:169[A]:ASN:HD22	1:A:172:ILE:HD12	1.63	0.64
3:F:181[A]:THR:HB	3:F:183[A]:ARG:HD2	1.74	0.64
2:E:61[B]:LYS:CE	12:E:2444:HOH:O	2.46	0.64
1:A:130:THR:HG23	12:A:3696[B]:HOH:O	1.97	0.64
1:D:36[A]:ARG:HD3	1:D:85:ASP:OD1	1.99	0.62
12:B:2205:HOH:O	2:E:188:PRO:HD3	1.99	0.62
1:D:429:LEU:CD1	3:F:234[B]:MET:HE1	2.30	0.61
2:E:122[B]:ASP:HB2	12:E:1158:HOH:O	2.00	0.61
3:F:177:TYR:CE2	3:F:179[A]:LYS:HG2	2.36	0.61
3:F:177:TYR:HE2	3:F:179[A]:LYS:HG2	1.66	0.60
2:E:61[B]:LYS:NZ	12:E:2444:HOH:O	2.27	0.60
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.31	0.60
3:F:181[A]:THR:O	3:F:183[A]:ARG:HG3	2.02	0.59
1:D:169:ASN:CG	1:D:172[A]:ILE:HG13	2.27	0.59
3:C:64[B]:ASP:HB2	12:C:3620:HOH:O	2.03	0.58
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:CG	2.51	0.58
2:B:27:LEU:HD21	2:B:246[B]:MET:HE1	1.82	0.58
1:A:24[A]:THR:CG2	12:C:3803:HOH:O	2.32	0.58
1:A:60:ILE:HD12	12:D:3878:HOH:O	2.03	0.58
3:F:44:ALA:HB1	3:F:45:PRO:HD2	1.88	0.56
1:D:169:ASN:OD1	1:D:172[A]:ILE:HG13	2.06	0.56
2:B:58:LYS:NZ	12:B:3633:HOH:O	2.27	0.55
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:HH11	1.72	0.55
2:B:299:LEU:HD21	12:C:1043:HOH:O	2.06	0.54
2:B:188:PRO:HD3	12:E:1304:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:LYS:NZ	12:D:3755[B]:HOH:O	2.25	0.54
1:A:383[A]:GLU:HG3	12:A:2606:HOH:O	2.07	0.53
2:B:3:LYS:HE2	2:B:234:GLU:OE1	2.08	0.53
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.09	0.53
2:B:424[A]:GLU:HG3	12:B:3930:HOH:O	2.08	0.53
3:C:64[A]:ASP:HB3	3:C:67[A]:ARG:HB3	1.90	0.53
3:F:182[A]:GLY:O	3:F:203:GLU:HG2	2.08	0.53
2:E:61[B]:LYS:HE3	12:E:2370:HOH:O	2.09	0.52
1:D:383[B]:GLU:HG2	1:D:387[B]:GLU:OE2	2.09	0.52
1:A:169[A]:ASN:ND2	1:A:172:ILE:CD1	2.71	0.52
3:F:57:GLU:HG2	12:F:939:HOH:O	2.08	0.52
1:A:178[A]:PRO:HD2	12:A:1652:HOH:O	2.11	0.51
2:E:17:LEU:HD21	2:E:20[A]:GLU:CG	2.40	0.50
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.93	0.50
1:A:432:TYR:HB3	3:C:234[B]:MET:HE3	1.86	0.50
3:C:194[B]:GLU:HG3	12:C:1318:HOH:O	2.11	0.50
1:D:45[B]:LYS:HE3	12:D:1271:HOH:O	2.11	0.50
3:F:181[A]:THR:CA	3:F:183[A]:ARG:HG3	2.42	0.50
2:E:27:LEU:HD21	2:E:246[B]:MET:HE1	1.94	0.49
2:B:58:LYS:NZ	2:B:58:LYS:HB3	2.27	0.49
2:B:119:ALA:HA	2:B:122[B]:ASP:OD2	2.11	0.49
1:A:443:PHE:CZ	6:A:554[A]:TP7:S7	3.06	0.49
2:E:342:THR:OG1	2:E:344[B]:LEU:HB2	2.12	0.49
2:B:261[B]:LYS:HG2	12:C:3925:HOH:O	2.12	0.48
3:C:182[B]:GLY:O	3:C:203:GLU:HG2	2.13	0.48
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	1.96	0.48
2:B:36:LYS:HA	2:E:123[B]:VAL:HG12	1.96	0.48
2:B:322:ARG:NH1	3:C:67[A]:ARG:HD3	2.29	0.48
2:B:27:LEU:HD22	2:B:246[B]:MET:SD	2.53	0.48
1:D:332:GLN:HA	1:D:335:THR:OG1	2.14	0.47
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:HG3	2.13	0.47
1:D:57:ASN:HB3	1:D:60[B]:ILE:HG12	1.96	0.47
1:D:172[A]:ILE:HD12	12:D:2242:HOH:O	2.14	0.47
2:B:113[A]:LEU:HB2	2:B:418:VAL:HG13	1.97	0.47
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.96	0.47
1:D:443:PHE:CZ	6:D:553[A]:TP7:S7	3.08	0.47
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CG	2.27	0.47
3:C:178[B]:ASN:HD21	3:C:180[B]:ASP:HB2	1.80	0.47
2:E:3[B]:LYS:NZ	2:E:234:GLU:OE1	2.43	0.47
1:A:328:VAL:HB	5:D:552:F43:H9A1	1.96	0.46
3:C:184[B]:VAL:N	3:C:202:GLY:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:83[A]:GLU:HG2	12:E:3720:HOH:O	2.14	0.46
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	1.97	0.46
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.97	0.46
2:E:119[B]:ALA:O	2:E:123[B]:VAL:HG22	2.16	0.46
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD3	2.46	0.46
1:A:269:VAL:HG12	12:A:1300:HOH:O	2.14	0.46
1:D:154:HIS:CE1	1:D:545:LEU:HD21	2.51	0.45
3:C:145:PRO:HB2	3:C:184[B]:VAL:HB	1.97	0.45
3:C:178[B]:ASN:HD22	3:C:178[B]:ASN:C	2.24	0.45
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.50	0.45
1:D:298[A]:GLU:HB2	12:D:1710:HOH:O	2.16	0.45
2:E:42[A]:ILE:HG13	2:E:425:PHE:CE1	2.52	0.45
2:B:236[C]:MET:HE2	2:B:303:ASN:CB	2.47	0.45
3:C:178[B]:ASN:HD22	3:C:180[B]:ASP:H	1.64	0.45
2:E:424[B]:GLU:HG3	12:E:3642:HOH:O	2.16	0.45
3:C:117:LEU:HB2	3:C:120:ARG:HG3	1.99	0.44
2:B:286:LYS:HE2	2:B:288:LEU:HD21	2.00	0.44
3:F:153[A]:LYS:NZ	12:F:1186:HOH:O	2.32	0.43
3:C:179[B]:LYS:CE	12:C:3001:HOH:O	2.65	0.43
1:A:352[A]:GLU:CG	12:A:4100:HOH:O	2.41	0.43
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.86	0.43
1:A:177[A]:ASP:HB2	12:A:2279:HOH:O	2.17	0.43
2:E:374:ILE:C	2:E:374:ILE:HD12	2.43	0.43
1:D:473:PRO:O	1:D:479:ALA:HA	2.19	0.43
2:E:236[A]:MET:HE2	2:E:236[A]:MET:HB3	1.80	0.43
1:A:118:LYS:HZ2	1:A:118:LYS:HG2	1.74	0.43
3:C:205:LEU:HD22	3:C:209:THR:HG21	1.99	0.43
2:B:362:PHE:O	2:B:369:GLY:HA3	2.18	0.42
1:D:60[B]:ILE:HA	1:D:60[B]:ILE:HD13	1.86	0.42
1:D:355[B]:GLU:OE2	1:D:355[B]:GLU:HA	2.19	0.42
2:E:113[B]:LEU:C	2:E:113[B]:LEU:HD23	2.44	0.42
2:B:236[C]:MET:HE2	2:B:303:ASN:HB2	2.00	0.42
3:F:59:MET:HB2	3:F:59:MET:HE2	1.47	0.42
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.77	0.42
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.55	0.42
1:A:332:GLN:HA	1:A:335:THR:OG1	2.18	0.42
2:B:342:THR:OG1	2:B:344[B]:LEU:HB2	2.19	0.42
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	2.01	0.42
2:E:61[B]:LYS:HE2	12:E:2444:HOH:O	2.14	0.42
2:E:199:HIS:CE1	2:E:415[B]:ILE:HD12	2.54	0.42
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179[B]:LYS:HE3	12:C:3001:HOH:O	2.19	0.42
2:E:317:ASN:O	3:F:111:GLY:HA2	2.20	0.42
2:E:362:PHE:O	2:E:369:GLY:HA3	2.20	0.42
2:E:39:VAL:HG21	2:E:221:THR:HG21	2.02	0.41
9:F:251:EDO:C2	12:F:832:HOH:O	2.68	0.41
1:A:387[B]:GLU:HG3	12:A:1069:HOH:O	2.19	0.41
2:B:257:LYS:HE2	12:B:3430:HOH:O	2.21	0.41
3:C:183[B]:ARG:HA	3:C:202:GLY:O	2.21	0.41
3:F:59:MET:O	3:F:60:ASP:C	2.62	0.41
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.55	0.41
2:E:196[B]:MET:O	2:E:197:VAL:C	2.64	0.41
3:C:63:GLU:HG3	3:C:68:GLU:OE2	2.21	0.41
2:B:39:VAL:HG21	2:B:221:THR:HG21	2.03	0.41
1:A:432:TYR:CB	3:C:234[B]:MET:CE	2.74	0.40
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.56	0.40
1:D:428:TYR:HD1	1:D:450:ASP:HB3	1.87	0.40
1:A:55:GLN:OE1	1:D:155:PRO:HB3	2.21	0.40
1:A:268:PRO:HG2	1:A:271:AGM:NH2	2.36	0.40
2:B:333:TYR:HB2	3:C:106:LEU:HD22	2.04	0.40
1:A:109:LEU:HB2	1:A:204[B]:ILE:HG23	2.03	0.40
2:B:246[A]:MET:HE3	2:B:429:LEU:CD1	2.49	0.40
2:B:283:LYS:HE2	2:B:297[B]:ASP:OD2	2.21	0.40
2:B:339:GLU:HG3	2:B:346:SER:HB3	2.02	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	570/549 (104%)	550 (96%)	19 (3%)	1 (0%)	43	17
1	D	571/549 (104%)	556 (97%)	14 (2%)	1 (0%)	43	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	465/442 (105%)	456 (98%)	9 (2%)	0	100	100
2	E	472/442 (107%)	461 (98%)	11 (2%)	0	100	100
3	C	264/248 (106%)	256 (97%)	8 (3%)	0	100	100
3	F	266/248 (107%)	261 (98%)	5 (2%)	0	100	100
All	All	2608/2478 (105%)	2540 (97%)	66 (2%)	2 (0%)	48	18

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	462/434 (106%)	455 (98%)	7 (2%)	57	21
1	D	462/434 (106%)	456 (99%)	6 (1%)	61	26
2	B	366/341 (107%)	362 (99%)	4 (1%)	65	33
2	E	372/341 (109%)	371 (100%)	1 (0%)	86	67
3	C	233/216 (108%)	231 (99%)	2 (1%)	70	42
3	F	235/216 (109%)	229 (97%)	6 (3%)	40	7
All	All	2130/1982 (108%)	2104 (99%)	26 (1%)	65	29

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	LYS
1	A	12[B]	LYS
1	A	118	LYS
1	A	123	GLU
1	A	126	PRO

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	450	ASP
2	B	3	LYS
2	B	58	LYS
2	B	97	GLU
2	B	185	LEU
3	C	61	GLU
3	C	150	VAL
1	D	36[A]	ARG
1	D	36[B]	ARG
1	D	122	LYS
1	D	352[A]	GLU
1	D	352[B]	GLU
1	D	450	ASP
2	E	58	LYS
3	F	61	GLU
3	F	150	VAL
3	F	179[A]	LYS
3	F	179[B]	LYS
3	F	186	MET
3	F	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	241	GLN
1	A	317	GLN
2	B	102	ASN
2	B	115	GLN
3	C	121	GLN
1	D	111	HIS
1	D	296	ASN
1	D	317	GLN
1	D	437	GLN
2	E	102	ASN
2	E	115	GLN
2	E	318	GLN
3	F	121	GLN
3	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGM	A	271	1	10,11,12	0.88	0	7,13,15	1.57	2 (28%)
1	GL3	A	445	1	2,3,4	1.89	1 (50%)	1,2,4	0.01	0
1	MGN	A	400	1	6,9,10	1.00	0	7,12,14	0.79	0
1	MHS	D	257	1	10,11,12	1.56	3 (30%)	5,14,16	9.36	5 (100%)
1	AGM	D	271	1	10,11,12	1.22	1 (10%)	7,13,15	1.18	0
1	GL3	D	445	1	2,3,4	2.06	1 (50%)	1,2,4	0.49	0
1	SMC	D	452	1	5,6,7	1.00	0	3,6,8	1.27	0
1	MHS	A	257	1	10,11,12	2.01	6 (60%)	5,14,16	8.60	3 (60%)
1	SMC	A	452	1	5,6,7	0.98	0	3,6,8	1.05	0
1	MGN	D	400	1	6,9,10	1.66	1 (16%)	7,12,14	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AGM	A	271	1	-	2/10/11/13	-
1	GL3	A	445	1	-	0/1/1/2	-
1	MGN	A	400	1	-	0/7/9/12	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	AGM	D	271	1	-	2/10/11/13	-
1	GL3	D	445	1	-	1/1/1/2	-
1	SMC	D	452	1	-	1/3/5/7	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	A	452	1	-	1/3/5/7	-
1	MGN	D	400	1	-	0/7/9/12	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CE1-NE2	3.28	1.40	1.32
1	D	400	MGN	CB1-CA	-3.16	1.51	1.55
1	D	445	GL3	C-S	-2.91	1.68	1.80
1	D	271	AGM	CD-NE1	2.83	1.53	1.46
1	A	257	MHS	CD2-CG	2.80	1.40	1.36
1	A	445	GL3	C-S	-2.64	1.69	1.80
1	A	257	MHS	CG-ND1	-2.37	1.34	1.38
1	D	257	MHS	CB-CG	2.30	1.54	1.49
1	D	257	MHS	CE1-NE2	2.29	1.38	1.32
1	D	257	MHS	CD2-NE2	-2.13	1.34	1.37
1	A	257	MHS	O-C	2.06	1.27	1.20
1	A	257	MHS	CE1-ND1	2.04	1.40	1.35
1	A	257	MHS	CM-ND1	2.02	1.50	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	ND1-CE1-NE2	-19.24	101.48	112.94
1	A	257	MHS	ND1-CE1-NE2	-18.29	102.05	112.94
1	D	257	MHS	CD2-NE2-CE1	6.72	114.02	105.24
1	A	257	MHS	CD2-NE2-CE1	4.27	110.83	105.24
1	A	257	MHS	CM-ND1-CE1	-3.90	118.99	126.28
1	D	257	MHS	CM-ND1-CE1	-3.46	119.81	126.28
1	D	257	MHS	CM-ND1-CG	2.59	129.45	126.69
1	A	271	AGM	NH1-CZ-NE1	2.47	125.03	119.58
1	A	271	AGM	CE2-CD-CG	2.21	115.51	111.48
1	D	257	MHS	CG-CD2-NE2	-2.07	105.39	109.79

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	452	SMC	CA-CB-SG-CS
1	A	452	SMC	CA-CB-SG-CS
1	D	445	GL3	S-C-CA-N

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Mol	Chain	Res	Type	Atoms
1	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	NE1-CD-CG-CB
1	D	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	271	AGM	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 10 are monoatomic - leaving 14 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	TPZ	D	555[B]	-	17,18,18	1.26	2 (11%)	22,24,24	1.17	1 (4%)
6	TP7	D	553[A]	-	19,20,20	0.92	1 (5%)	24,26,26	1.11	2 (8%)
9	EDO	F	251	-	3,3,3	0.65	0	2,2,2	0.42	0
9	EDO	F	252	-	3,3,3	0.65	0	2,2,2	0.25	0
11	PEG	C	1	-	6,6,6	0.54	0	5,5,5	1.25	1 (20%)
9	EDO	C	251	-	3,3,3	0.61	0	2,2,2	0.93	0
6	TP7	A	554[A]	-	19,20,20	0.95	1 (5%)	24,26,26	1.32	2 (8%)
8	TPZ	A	556[B]	-	17,18,18	1.15	1 (5%)	22,24,24	1.39	2 (9%)
9	EDO	D	556	-	3,3,3	0.55	0	2,2,2	0.55	0
5	F43	D	552	1,7	63,71,71	2.64	19 (30%)	73,118,118	1.93	26 (35%)
9	EDO	A	557	-	3,3,3	0.52	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	F43	A	1	1,7	63,71,71	2.59	14 (22%)	73,118,118	1.68	21 (28%)
7	COM	A	555	5	6,6,6	2.03	1 (16%)	8,8,8	1.60	2 (25%)
7	COM	D	554	5	6,6,6	1.98	1 (16%)	8,8,8	1.35	3 (37%)

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
8	TPZ	D	555[B]	-	-	1/22/22/22	-
6	TP7	D	553[A]	-	-	3/24/24/24	-
9	EDO	F	251	-	-	1/1/1/1	-
9	EDO	F	252	-	-	1/1/1/1	-
11	PEG	C	1	-	-	2/4/4/4	-
9	EDO	C	251	-	-	0/1/1/1	-
6	TP7	A	554[A]	-	-	3/24/24/24	-
8	TPZ	A	556[B]	-	-	1/22/22/22	-
9	EDO	D	556	-	-	1/1/1/1	-
5	F43	D	552	1,7	-	11/28/185/185	-
9	EDO	A	557	-	-	0/1/1/1	-
5	F43	A	1	1,7	-	10/28/185/185	-
7	COM	A	555	5	-	0/4/4/4	-
7	COM	D	554	5	-	0/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	NI-NB	10.31	2.14	1.89
5	D	552	F43	NI-NA	8.90	2.10	1.89
5	D	552	F43	NI-NB	8.81	2.10	1.89
5	A	1	F43	NI-ND	7.96	2.08	1.89
5	D	552	F43	NI-ND	7.82	2.08	1.89
5	A	1	F43	NI-NA	7.11	2.06	1.89
5	A	1	F43	CHA-C4D	6.64	1.59	1.53
5	A	1	F43	CHB-C1B	-6.63	1.48	1.53
5	D	552	F43	CHB-C1B	5.59	1.57	1.53
5	D	552	F43	CHD-C1D	5.52	1.52	1.43
7	A	555	COM	C2-S2	-4.48	1.71	1.77
7	D	554	COM	C2-S2	-4.24	1.71	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	OEB-CCB	-3.95	1.17	1.30
5	D	552	F43	C6D-C7D	-3.48	1.46	1.50
5	D	552	F43	C1D-ND	-3.21	1.23	1.30
5	D	552	F43	OEB-CCB	-3.03	1.20	1.30
5	D	552	F43	CHC-C4B	2.89	1.47	1.39
8	D	555[B]	TPZ	O-C	2.75	1.30	1.22
5	A	1	F43	CHC-C4B	2.72	1.46	1.39
5	D	552	F43	C5C-C2C	2.70	1.57	1.53
5	D	552	F43	O8D-C7D	2.62	1.28	1.23
5	D	552	F43	C3C-C4C	2.58	1.54	1.50
5	D	552	F43	C8B-C6B	2.47	1.56	1.50
5	D	552	F43	CHA-C4D	-2.43	1.50	1.53
5	D	552	F43	OBD-CAD	2.34	1.29	1.22
8	D	555[B]	TPZ	C5-S5	2.33	1.89	1.80
5	D	552	F43	C8C-C3C	2.30	1.58	1.54
5	A	1	F43	C4A-NA	2.25	1.52	1.49
5	A	1	F43	C4D-ND	-2.25	1.45	1.49
5	D	552	F43	CAA-C3A	2.21	1.57	1.53
6	A	554[A]	TP7	O-C	-2.21	1.23	1.30
5	A	1	F43	C9B-C2B	2.21	1.58	1.54
5	A	1	F43	CAA-CBA	2.16	1.59	1.52
6	D	553[A]	TP7	OXT-C	2.14	1.28	1.22
8	A	556[B]	TPZ	OXT-C	-2.14	1.23	1.30
5	A	1	F43	C4C-NC	2.13	1.39	1.35
5	D	552	F43	CHC-C1C	-2.09	1.32	1.36
5	A	1	F43	C3C-C4C	2.09	1.54	1.50
5	A	1	F43	ODA-CCA	-2.05	1.24	1.30
5	D	552	F43	CHD-C7D	-2.01	1.41	1.45

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	552	F43	C2D-C1D-CHD	-5.74	114.73	121.85
5	D	552	F43	C5D-C2D-C1D	4.74	116.62	110.43
5	D	552	F43	C6D-C7D-CHD	4.58	125.39	116.94
5	D	552	F43	C1D-CHD-C4C	-4.27	113.29	125.28
5	A	1	F43	C3A-C2A-C1A	-3.95	96.02	99.97
5	A	1	F43	OBC-CAC-C9C	3.57	125.27	114.00
8	A	556[B]	TPZ	C3-C4-C5	-3.52	106.82	113.09
5	A	1	F43	C5D-C2D-C1D	3.50	115.00	110.43
5	A	1	F43	C3B-C4B-CHC	-3.46	115.97	123.33
5	A	1	F43	C1B-C2B-C3B	3.27	106.27	101.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	552	F43	OBC-CAC-C9C	3.23	124.20	114.00
5	D	552	F43	ODB-CCB-CBB	-3.18	113.02	123.09
5	D	552	F43	C2B-C1B-NB	3.17	106.57	101.86
5	A	1	F43	ODB-CCB-CBB	-3.17	113.02	123.09
5	D	552	F43	O8D-C7D-C6D	-3.17	115.67	120.87
5	A	1	F43	C4A-NA-C1A	-3.17	104.78	109.08
5	D	552	F43	C3A-C2A-C1A	3.16	103.14	99.97
7	A	555	COM	O3S-S2-O2S	-3.05	103.77	111.40
5	D	552	F43	C7D-CHD-C4C	3.03	128.11	121.76
8	A	556[B]	TPZ	CB-CA-N	3.01	118.05	111.54
5	A	1	F43	C9A-C2A-C3A	2.79	117.00	112.99
8	D	555[B]	TPZ	CB-CA-N	2.79	117.57	111.54
5	A	1	F43	O8D-C7D-C6D	-2.71	116.43	120.87
5	D	552	F43	C9A-C2A-C3A	2.70	116.87	112.99
5	A	1	F43	CAB-C3B-C2B	-2.67	113.10	119.00
5	D	552	F43	CAB-C3B-C2B	-2.65	113.15	119.00
6	A	554[A]	TP7	CB-CA-N	2.65	117.27	111.54
5	A	1	F43	C2C-C5C-C6C	-2.53	109.21	113.95
5	A	1	F43	OCC-CAC-C9C	-2.49	115.20	123.09
5	A	1	F43	O7C-C6C-C5C	-2.47	115.27	122.84
7	A	555	COM	O2S-S2-C2	2.38	110.33	106.73
5	D	552	F43	O8D-C7D-CHD	-2.35	118.94	122.77
5	A	1	F43	OEA-CCA-CBA	-2.35	115.64	123.09
5	D	552	F43	O8C-C6C-C5C	2.33	121.25	114.00
11	C	1	PEG	C3-O2-C2	2.30	123.34	113.26
6	D	553[A]	TP7	O4P-P-O1P	-2.30	101.13	109.33
5	D	552	F43	CHA-C4D-C3D	-2.27	111.51	117.90
6	A	554[A]	TP7	O4P-P-O1P	-2.25	101.33	109.33
5	A	1	F43	C3D-C4D-ND	2.25	105.83	102.34
5	D	552	F43	C2A-C3A-C4A	-2.21	99.02	102.36
5	D	552	F43	C4D-ND-C1D	2.19	111.73	108.46
5	D	552	F43	OBC-CAC-OCC	-2.16	117.77	123.33
5	A	1	F43	O8C-C6C-C5C	2.15	120.68	114.00
5	A	1	F43	CHA-C4D-C3D	-2.14	111.86	117.90
5	D	552	F43	C5C-C2C-C3C	-2.12	109.81	115.05
5	D	552	F43	O7C-C6C-C5C	-2.12	116.34	122.84
5	D	552	F43	CHC-C1C-NC	2.11	127.80	124.39
5	A	1	F43	C2B-C3B-C4B	-2.10	99.29	101.64
6	D	553[A]	TP7	CB-CA-N	2.09	116.06	111.54
5	D	552	F43	OCD-CAD-C9D	2.09	120.49	114.00
5	A	1	F43	CHC-C1C-NC	2.07	127.74	124.39
5	D	552	F43	OEB-CCB-ODB	2.07	128.65	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	F43	C6D-C5D-C2D	-2.07	107.33	111.45
5	A	1	F43	OEB-CCB-CBB	2.06	120.52	114.00
5	D	552	F43	O7A-C6A-C5A	-2.05	115.64	121.98
7	D	554	COM	O2S-S2-C2	2.04	109.82	106.73
7	D	554	COM	O1S-S2-C2	2.04	109.81	106.73
5	D	552	F43	C3D-C2D-C1D	-2.03	98.89	102.47
5	D	552	F43	C2C-C5C-C6C	-2.02	110.16	113.95
7	D	554	COM	O3S-S2-O2S	-2.02	106.35	111.40

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	552	F43	C3A-CAA-CBA-CCA
11	C	1	PEG	O1-C1-C2-O2
5	A	1	F43	C3A-CAA-CBA-CCA
11	C	1	PEG	O2-C3-C4-O4
9	F	251	EDO	O1-C1-C2-O2
6	D	553[A]	TP7	C2-C3-C4-C5
9	D	556	EDO	O1-C1-C2-O2
6	A	554[A]	TP7	C2-C3-C4-C5
5	A	1	F43	C2C-C5C-C6C-O7C
5	D	552	F43	C2C-C5C-C6C-O7C
5	D	552	F43	C2C-C5C-C6C-O8C
5	D	552	F43	CAA-CBA-CCA-OEA
5	A	1	F43	CAA-CBA-CCA-OEA
9	F	252	EDO	O1-C1-C2-O2
5	A	1	F43	CAB-CBB-CCB-OEB
5	D	552	F43	CAA-CBA-CCA-ODA
5	D	552	F43	CAB-CBB-CCB-OEB
5	A	1	F43	CAA-CBA-CCA-ODA
5	A	1	F43	CAB-CBB-CCB-ODB
5	D	552	F43	CAB-CBB-CCB-ODB
5	A	1	F43	C2C-C5C-C6C-O8C
8	A	556[B]	TPZ	C3-C4-C5-S5
8	D	555[B]	TPZ	C3-C4-C5-S5
6	A	554[A]	TP7	CB-O4P-P-O3P
6	D	553[A]	TP7	CB-O4P-P-O3P
5	D	552	F43	C8C-C9C-CAC-OBC
5	A	1	F43	C8C-C9C-CAC-OCC
6	A	554[A]	TP7	C4-C5-C6-C7
5	A	1	F43	C3D-C9D-CAD-OCD

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Mol	Chain	Res	Type	Atoms
5	D	552	F43	C3D-C9D-CAD-OCD
5	D	552	F43	C8C-C9C-CAC-OCC
5	A	1	F43	C8C-C9C-CAC-OBC
6	D	553[A]	TP7	C4-C5-C6-C7
5	D	552	F43	C3D-C9D-CAD-OB

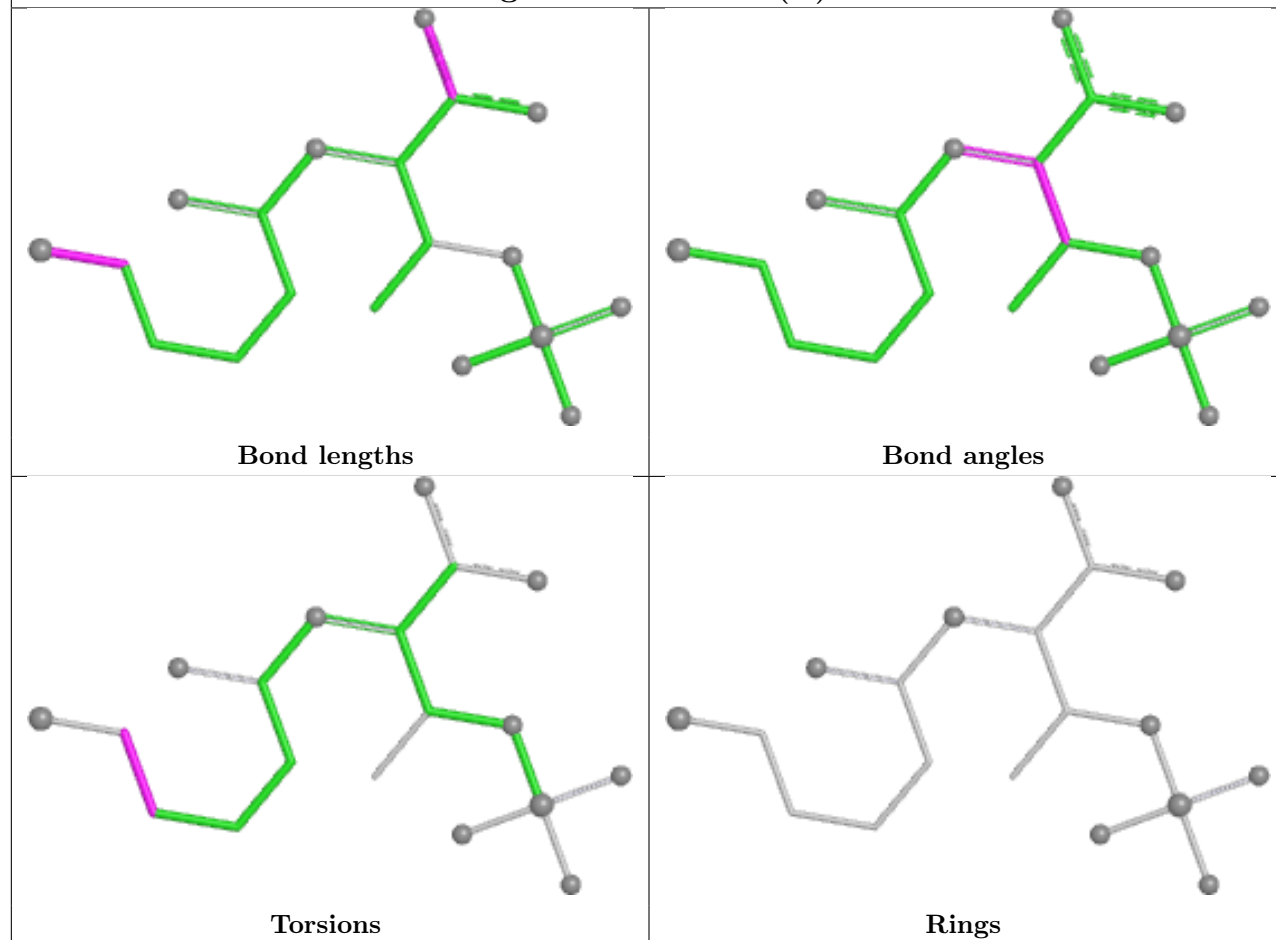
There are no ring outliers.

5 monomers are involved in 5 short contacts:

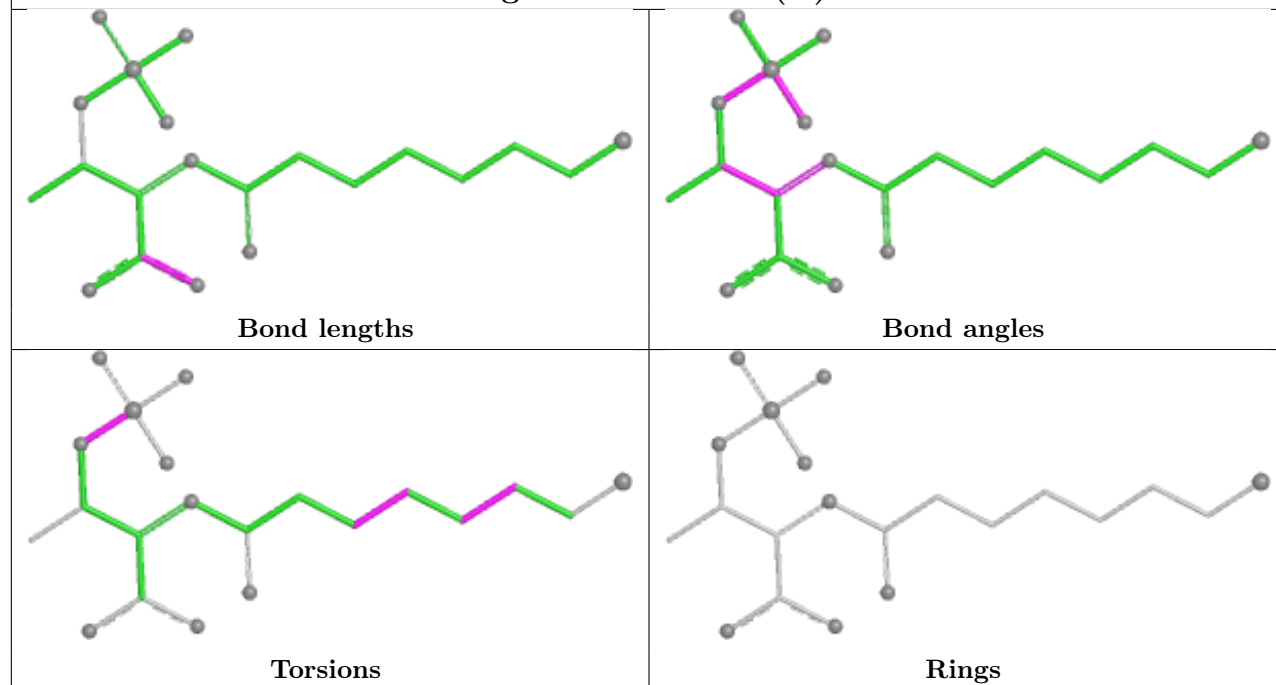
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	553[A]	TP7	1	0
9	F	251	EDO	1	0
6	A	554[A]	TP7	1	0
5	D	552	F43	1	0
5	A	1	F43	1	0

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.

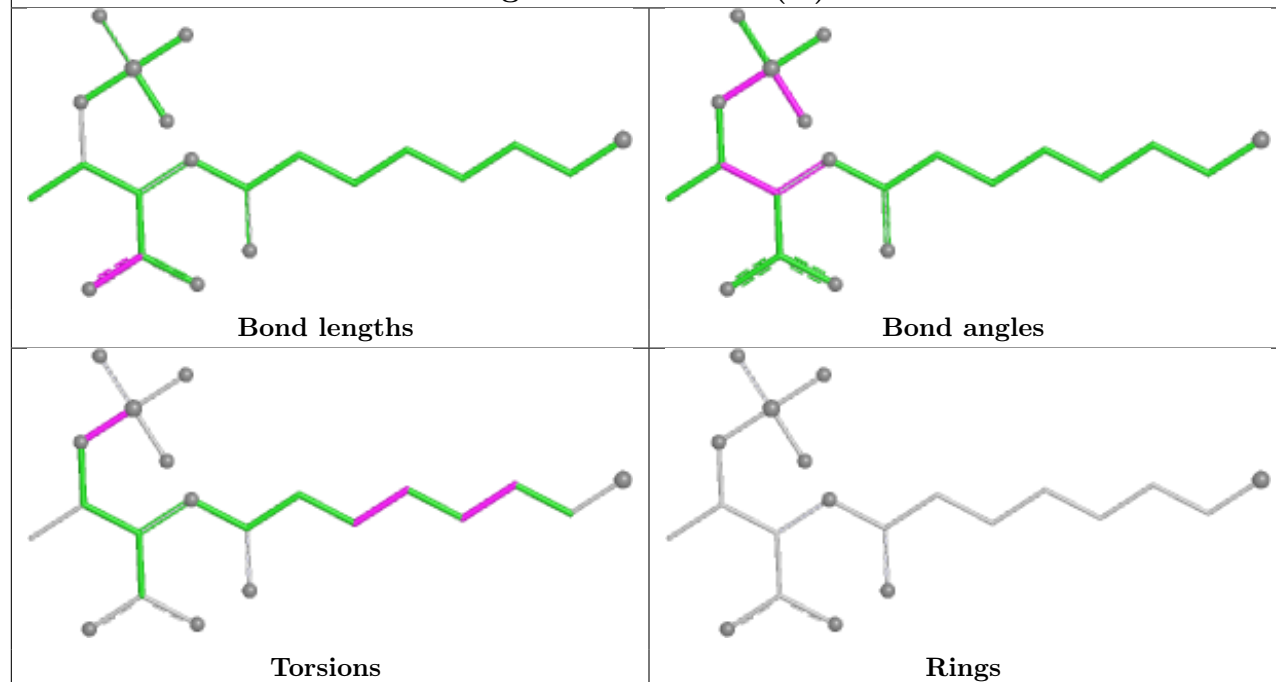
Ligand TPZ D 555 (B)



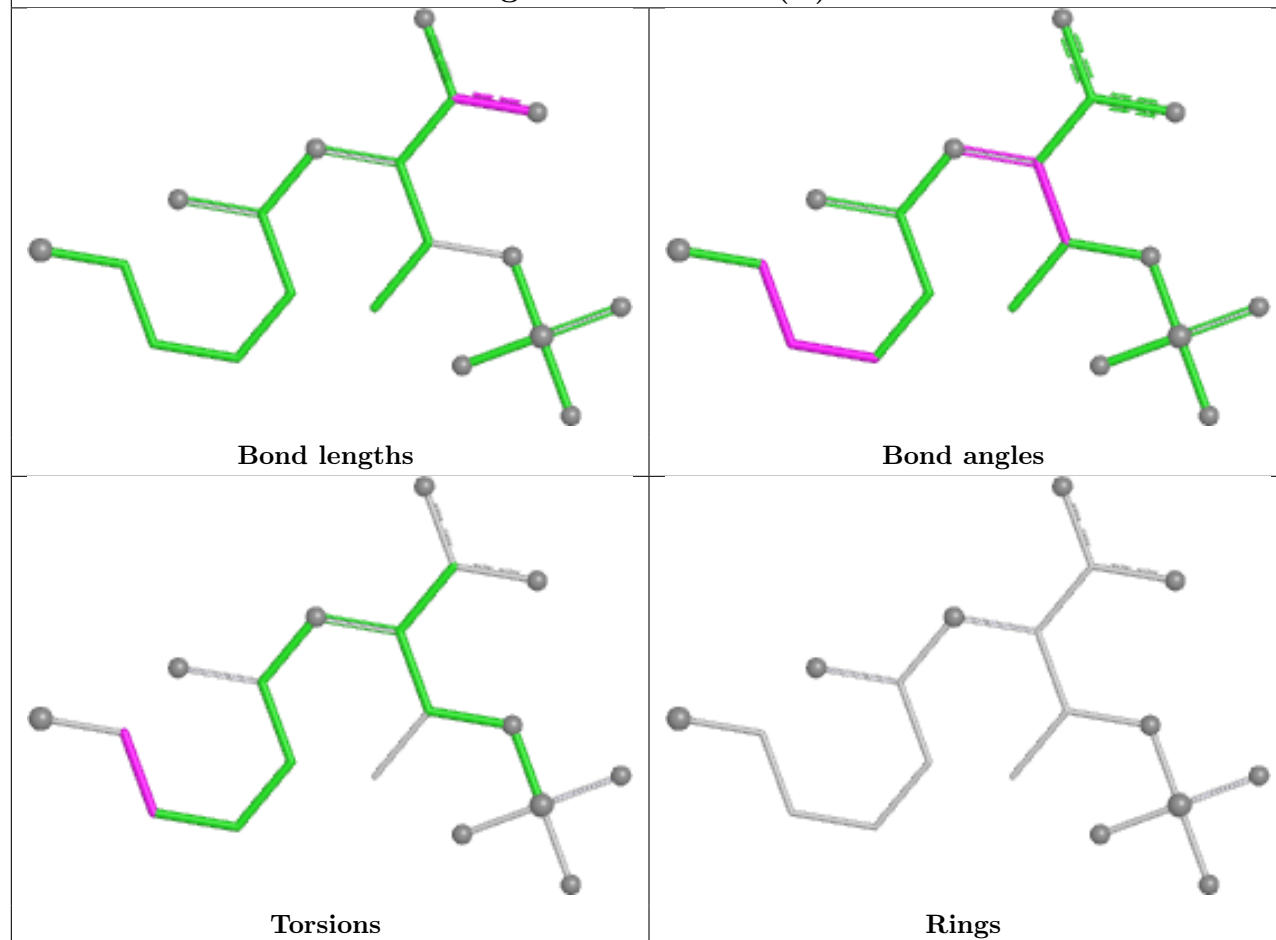
Ligand TP7 D 553 (A)



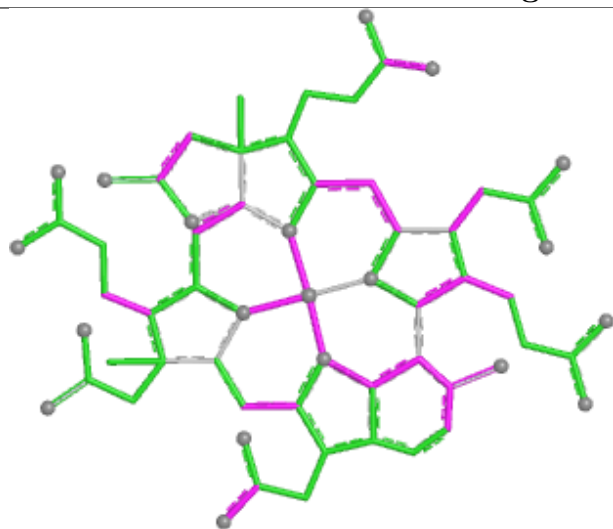
Ligand TP7 A 554 (A)



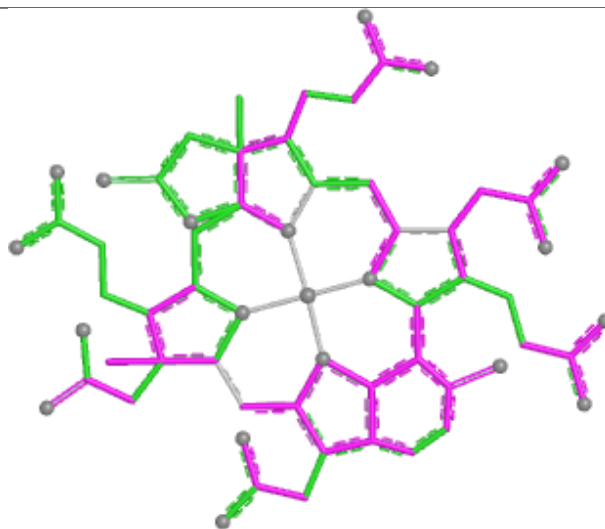
Ligand TPZ A 556 (B)



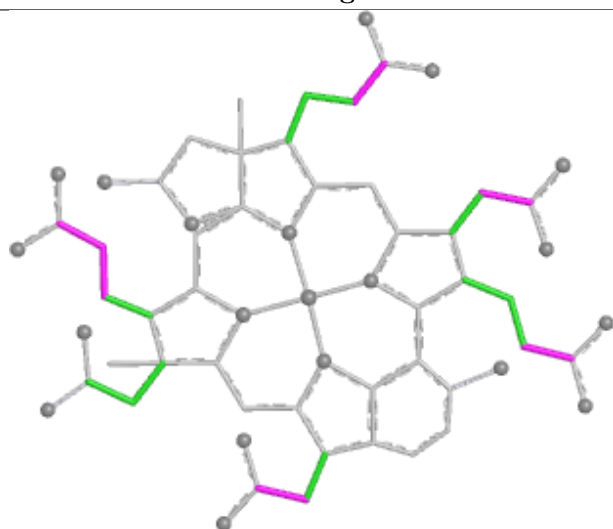
Ligand F43 D 552



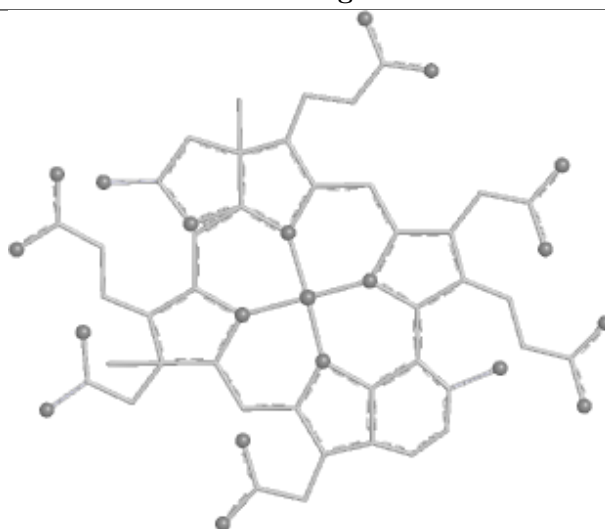
Bond lengths



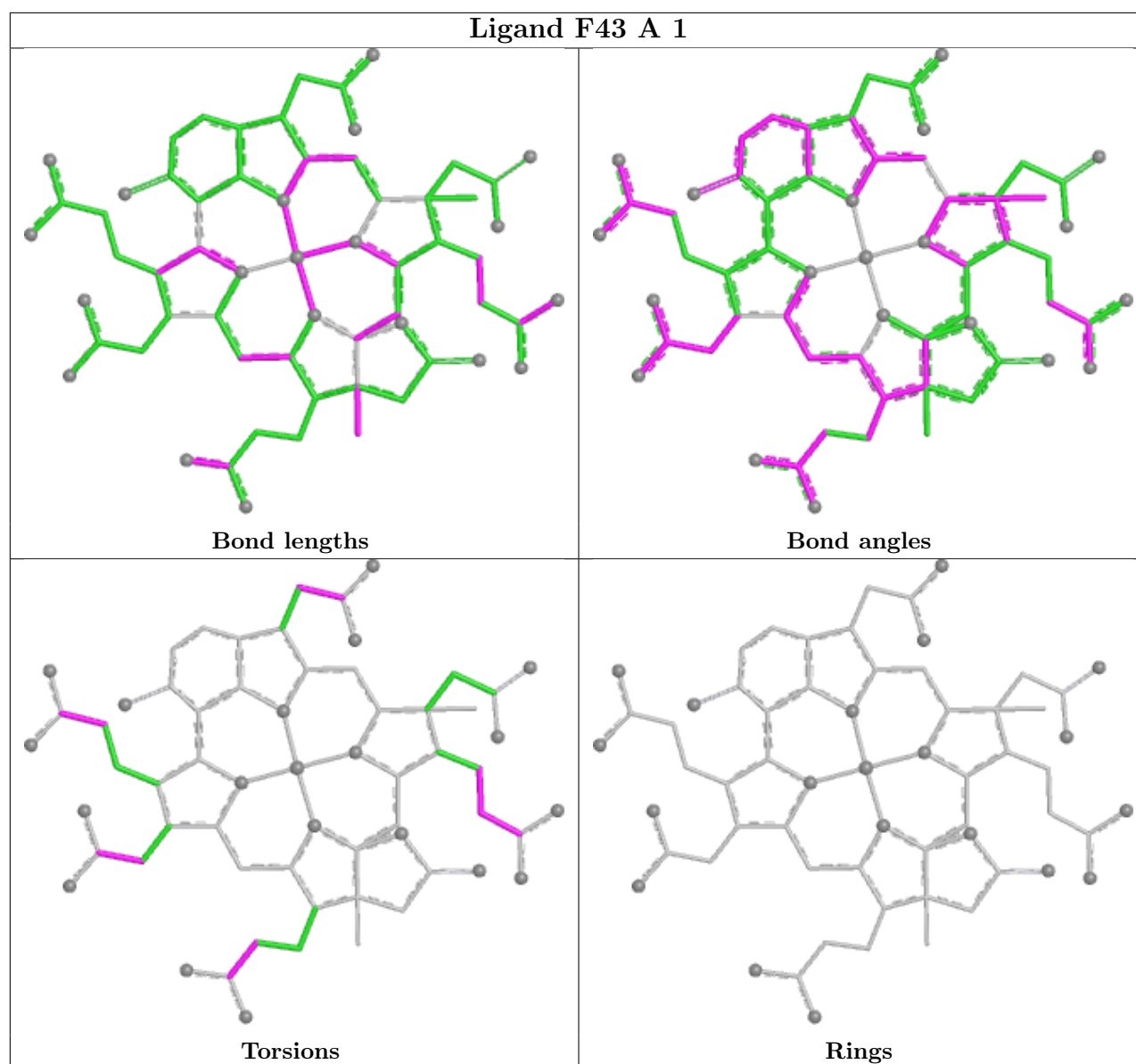
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/549 (98%)	-0.53	2 (0%) 88 91	3, 9, 19, 34	29 (5%)
1	D	543/549 (98%)	-0.52	3 (0%) 85 89	3, 9, 19, 37	30 (5%)
2	B	442/442 (100%)	-0.45	1 (0%) 91 93	5, 11, 19, 37	24 (5%)
2	E	442/442 (100%)	-0.39	1 (0%) 91 93	5, 11, 22, 38	31 (7%)
3	C	246/248 (99%)	-0.13	4 (1%) 70 74	6, 13, 27, 42	20 (8%)
3	F	246/248 (99%)	-0.04	6 (2%) 59 65	5, 13, 30, 51	22 (8%)
All	All	2462/2478 (99%)	-0.40	17 (0%) 84 88	3, 10, 21, 51	156 (6%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	549	ALA	4.0
1	D	118	LYS	3.2
3	F	181[A]	THR	3.0
3	F	45	PRO	2.9
1	D	2	ALA	2.8
3	F	60	ASP	2.7
2	E	441	ASN	2.7
3	C	45	PRO	2.6
2	B	98	ASP	2.6
3	F	57	GLU	2.5
3	C	62	PRO	2.4
3	C	46	GLY	2.4
3	F	59	MET	2.3
3	C	247	ASN	2.2
1	A	171	GLU	2.1
1	A	61	GLY	2.1
3	F	62	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MHS	A	257	11/12	0.97	0.05	8,9,12,15	0
1	MHS	D	257	11/12	0.97	0.04	8,9,11,13	0
1	MGN	A	400	10/11	0.98	0.04	6,7,9,9	0
1	AGM	D	271	12/13	0.98	0.04	5,6,7,8	0
1	MGN	D	400	10/11	0.98	0.03	6,7,7,8	0
1	SMC	A	452	7/8	0.99	0.04	6,7,8,9	0
1	AGM	A	271	12/13	0.99	0.03	5,6,6,7	0
1	SMC	D	452	7/8	0.99	0.04	6,7,8,9	0
1	GL3	D	445	4/5	1.00	0.02	5,6,6,7	0
1	GL3	A	445	4/5	1.00	0.04	6,7,7,7	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(Å ²)	Q<0.9
9	EDO	C	251	4/4	0.83	0.11	34,35,36,40	0
11	PEG	C	1	7/7	0.85	0.14	35,37,43,43	0
9	EDO	F	251	4/4	0.89	0.11	32,32,34,35	0
9	EDO	D	556	4/4	0.89	0.08	28,32,39,40	0
9	EDO	F	252	4/4	0.90	0.14	41,44,44,48	0
9	EDO	A	557	4/4	0.91	0.09	27,33,39,40	0
6	TP7	A	554[A]	21/21	0.94	0.06	4,7,10,21	21
6	TP7	D	553[A]	21/21	0.94	0.05	5,7,9,23	21
4	MG	A	551	1/1	0.95	0.10	15,15,15,15	1
4	MG	B	444	1/1	0.95	0.11	21,21,21,21	0
4	MG	A	553[B]	1/1	0.97	0.04	13,13,13,13	1
4	MG	C	250	1/1	0.97	0.06	17,17,17,17	0

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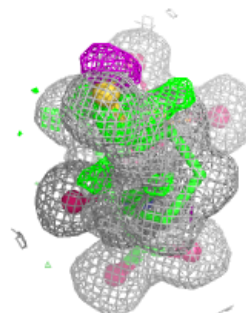
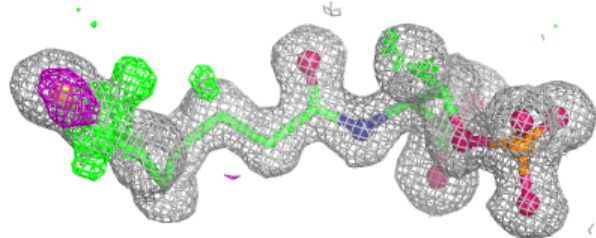
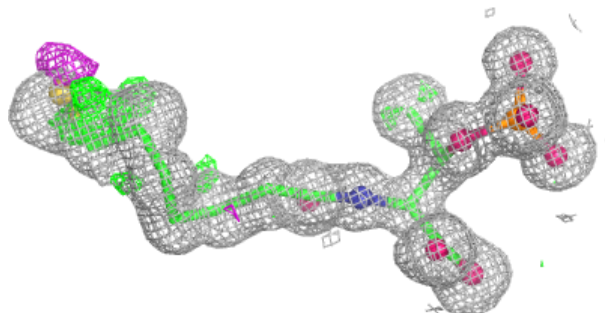
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	552[A]	1/1	0.98	0.15	17,17,17,17	1
4	MG	D	1	1/1	0.98	0.08	14,14,14,14	0
4	MG	E	444	1/1	0.98	0.17	24,24,24,24	0
4	MG	F	250	1/1	0.98	0.07	15,15,15,15	0
8	TPZ	D	555[B]	19/19	0.99	0.03	6,7,11,12	19
5	F43	D	552	62/62	0.99	0.03	6,8,9,12	0
4	MG	D	551	1/1	0.99	0.13	19,19,19,19	0
5	F43	A	1	62/62	0.99	0.03	5,7,9,11	0
7	COM	A	555	7/7	0.99	0.05	9,11,11,12	0
7	COM	D	554	7/7	0.99	0.05	7,9,11,11	0
10	ZN	A	558	1/1	0.99	0.03	10,10,10,10	1
8	TPZ	A	556[B]	19/19	0.99	0.04	6,7,11,12	19

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

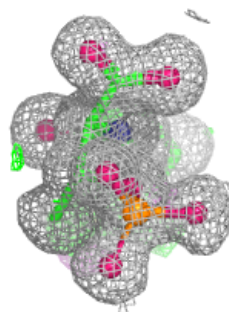
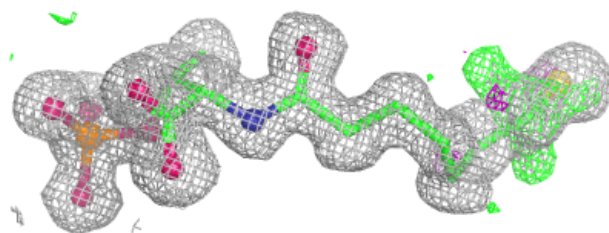
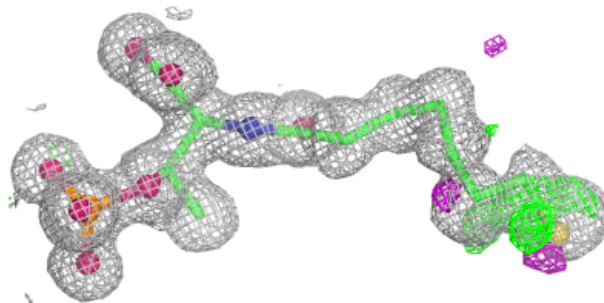
Electron density around TP7 A 554 (A):

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

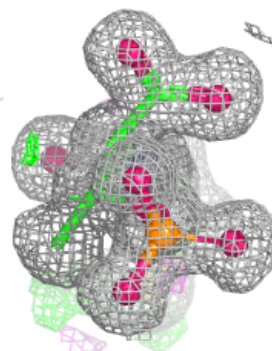
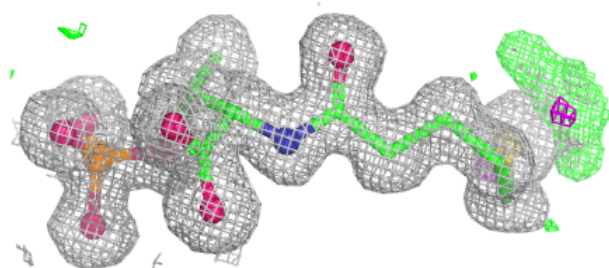
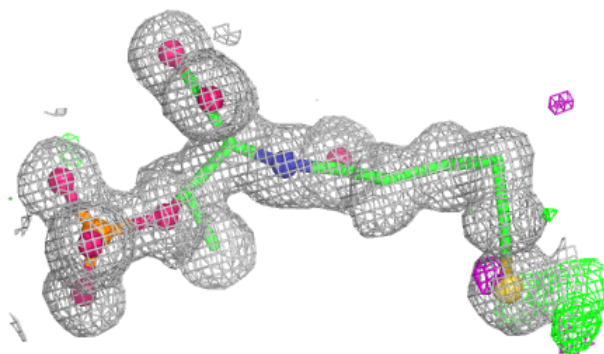


Electron density around TP7 D 553 (A):

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

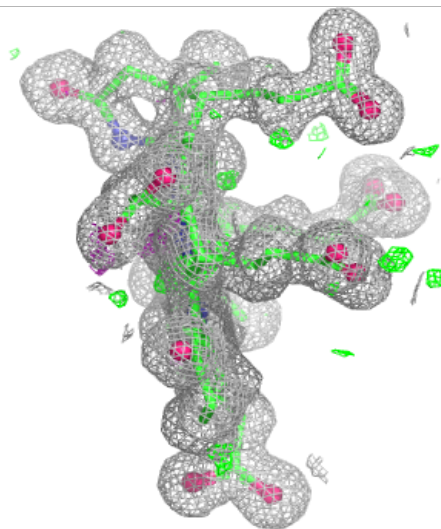
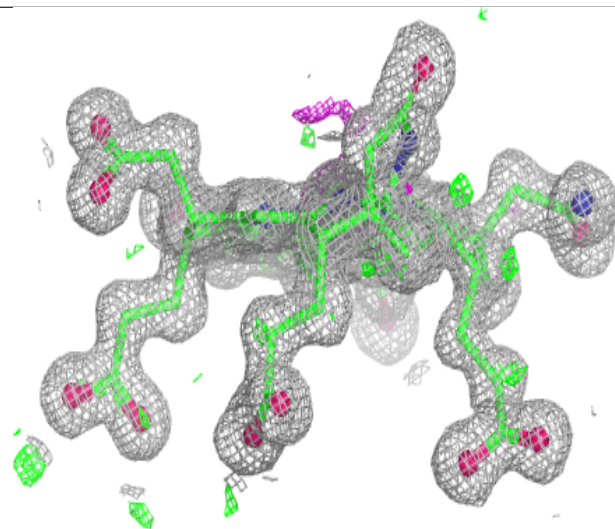
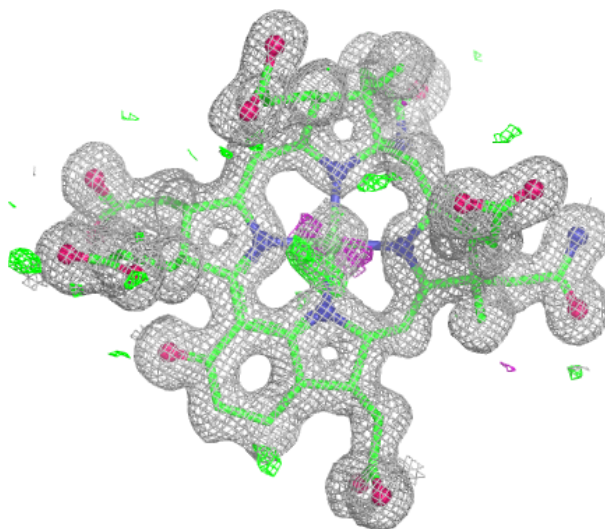
**Electron density around TPZ D 555 (B):**

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



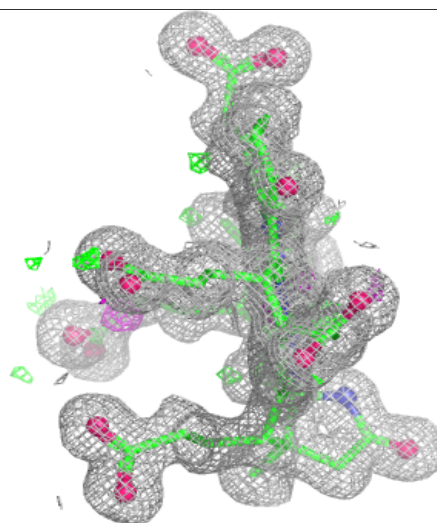
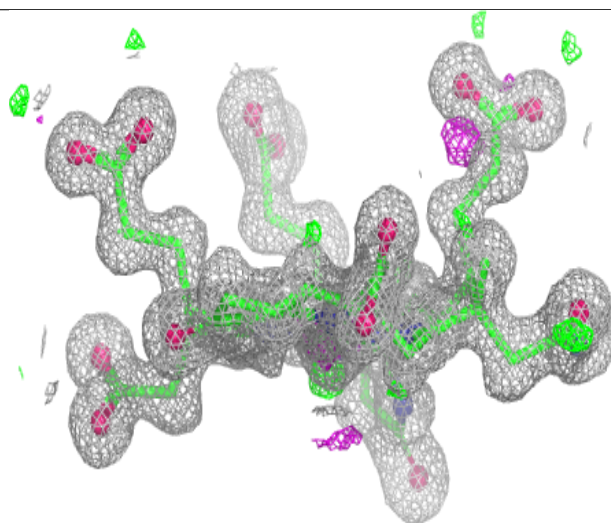
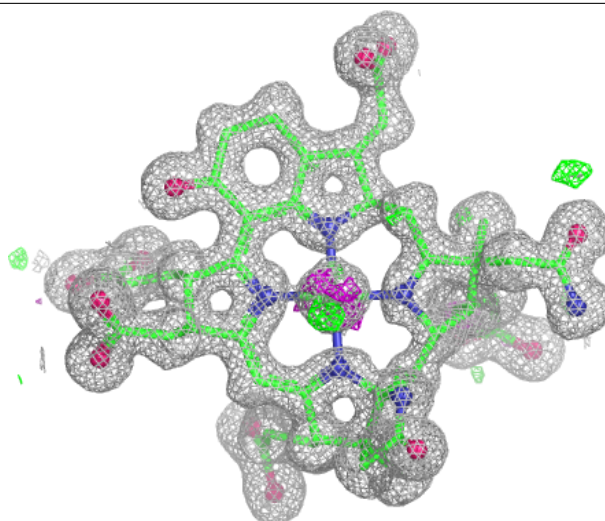
Electron density around F43 D 552:

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



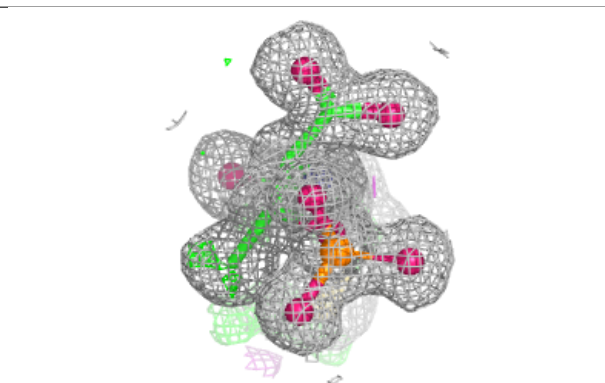
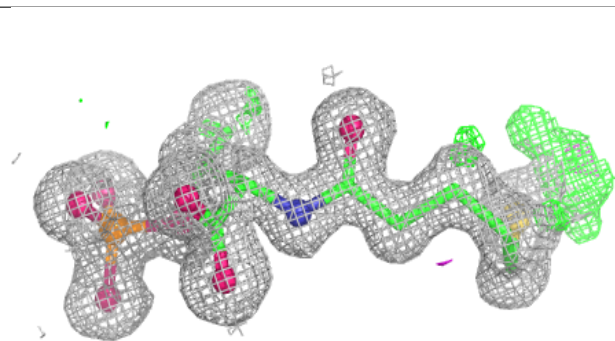
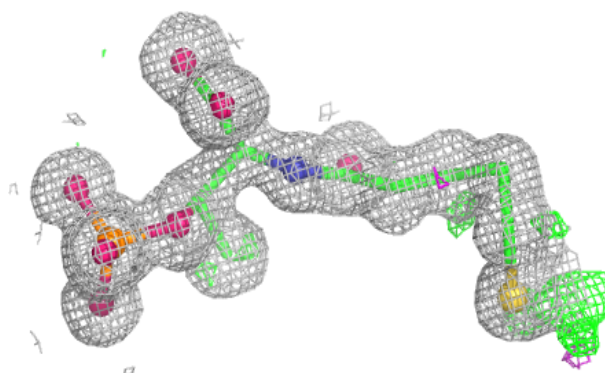
Electron density around F43 A 1:

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



Electron density around TPZ A 556 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.