Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 10:42 PM EDT

PDB ID	:	3M2V / pdb_00003m2v
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	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

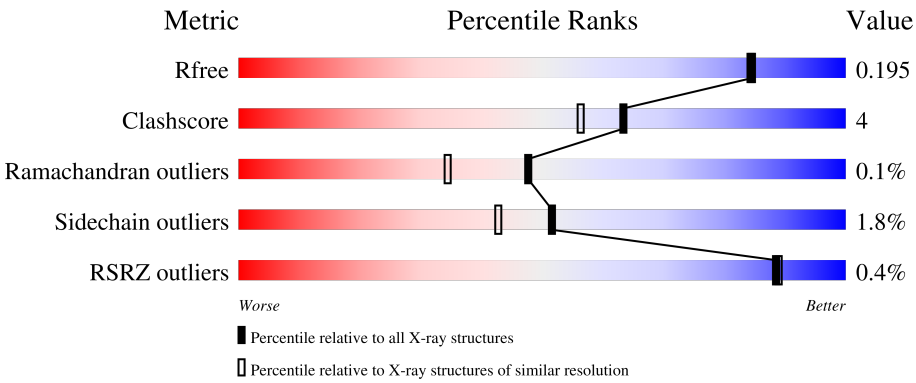
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	549	88% 12% •
1	D	549	84% 15% •
2	B	442	86% 13% •
2	E	442	% 88% 12%
3	C	248	88% 10% •

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Mol	Chain	Length	Quality of chain
3	F	248	2% 84% 14%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21893 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methyl-coenzyme M reductase I subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4408	2785	731	871	21	0	23	0
1	D	548	4359	2767	721	851	20	0	19	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	442	3422	2177	559	664	22	0	18	0
2	E	442	3431	2182	563	665	21	0	19	0

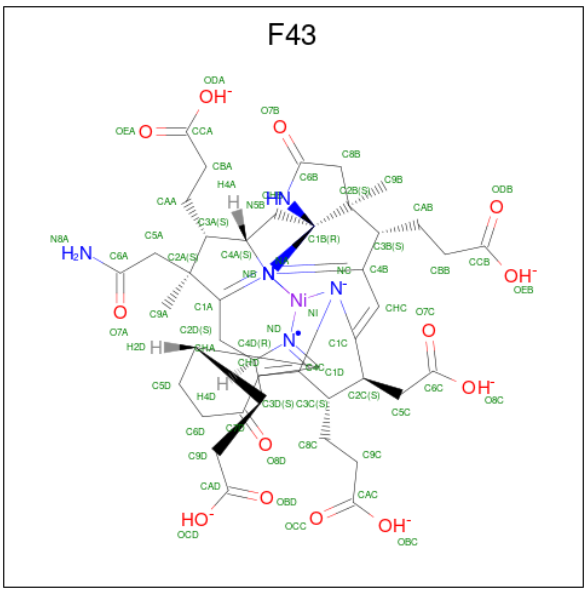
- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	248	2059	1273	362	412	12	0	8	0
3	F	247	2071	1280	367	412	12	0	11	0

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

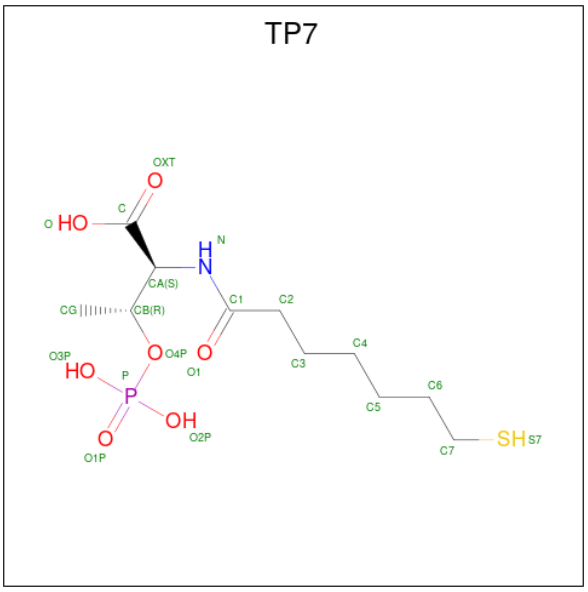
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	2	2	2	0	0
4	C	1	1	1	0	0
4	F	1	1	1	0	0

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



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

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



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

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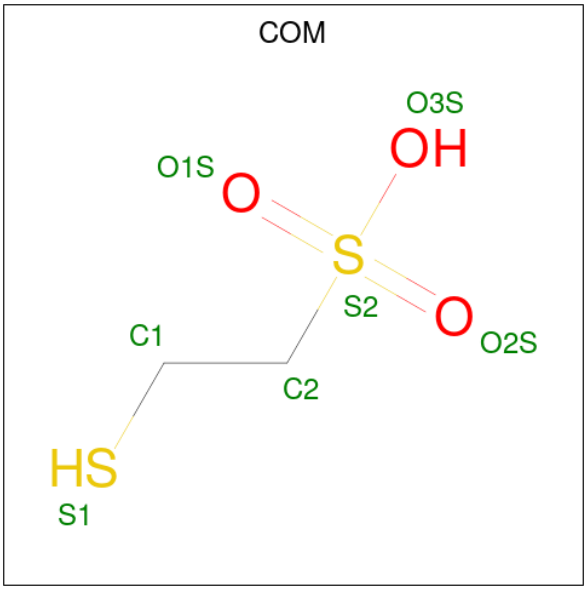
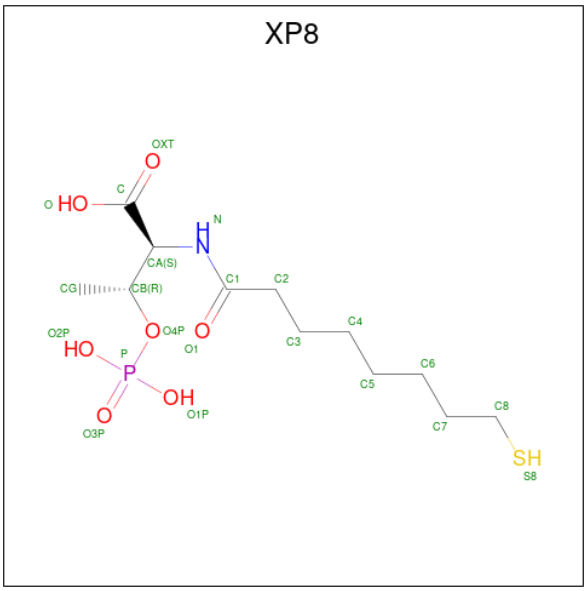
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	D	1	21	11	1	7	1	1	0	1

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



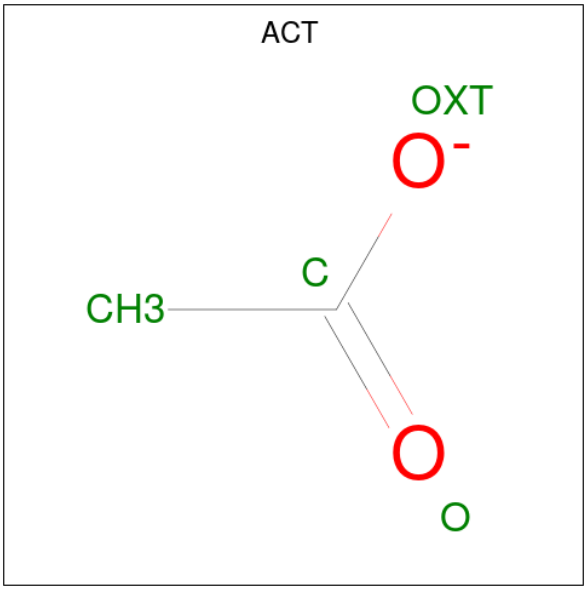
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
7	A	1	7	2	3	2	0	0
			Total	C	O	S		
7	D	1	7	2	3	2	0	0

- Molecule 8 is O-phosphono-N-(8-sulfanyloctanoyl)-L-threonine (CCD ID: XP8) (formula: $C_{12}H_{24}NO_7PS$).



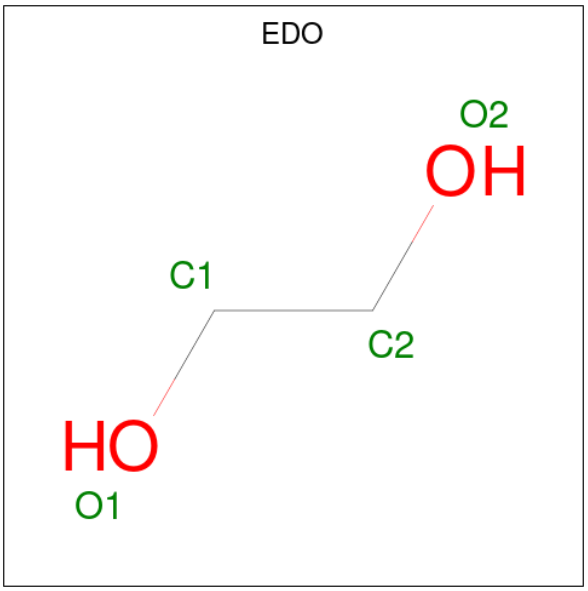
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
8	A	1	22	12	1	7	1	1	0	1
			Total	C	N	O	P	S		
8	D	1	22	12	1	7	1	1	0	1

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



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

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



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

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	427	435	435	0	15
			Total	O		
12	B	345	349	349	0	5
			Total	O		
12	C	200	201	201	0	8
			Total	O		
12	D	415	421	421	0	9

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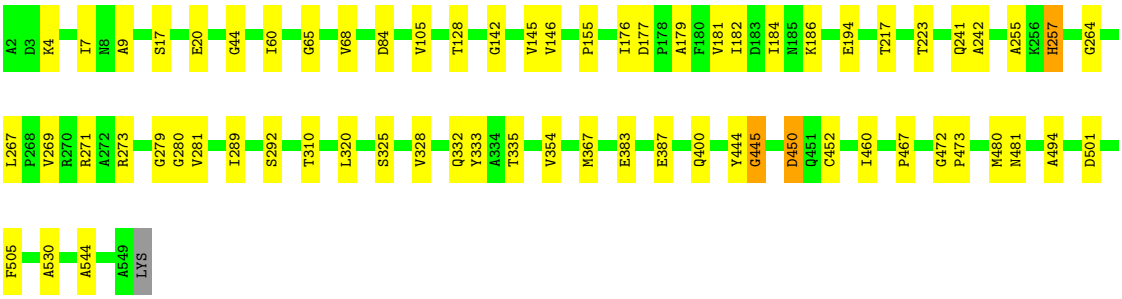
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	E	312	314	314	0	6
			Total	O		
12	F	172	173	173	0	6

3 Residue-property plots (i)

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

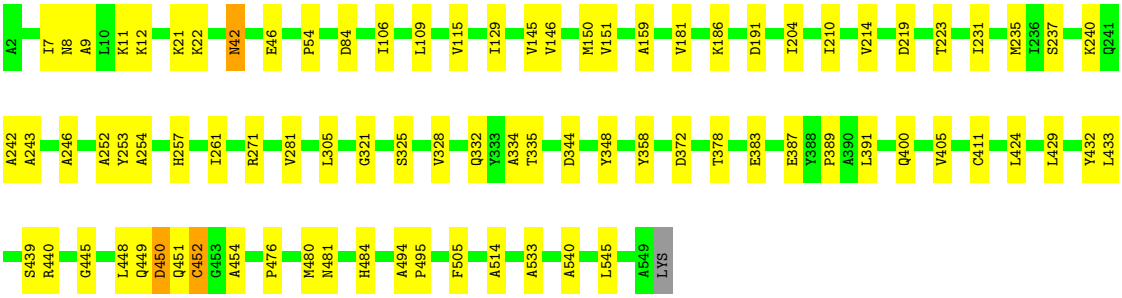
• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain A:



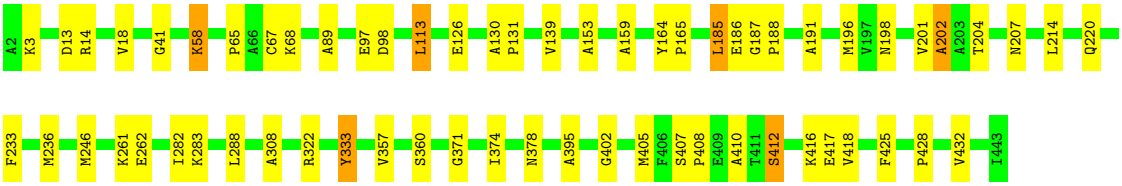
• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain D:



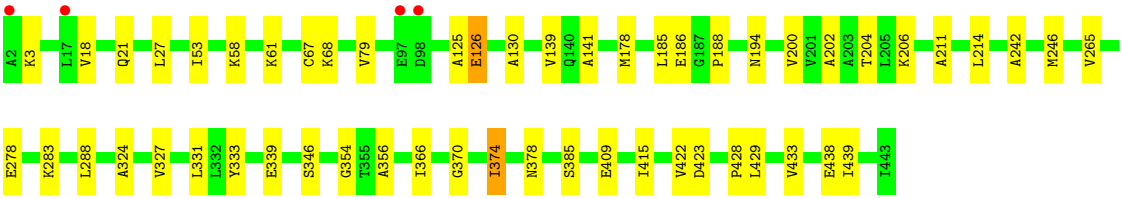
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain B:



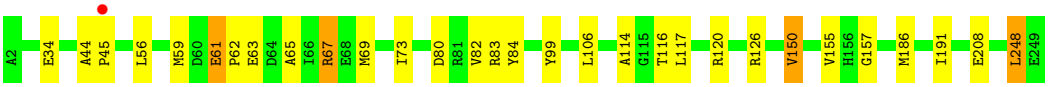
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E:



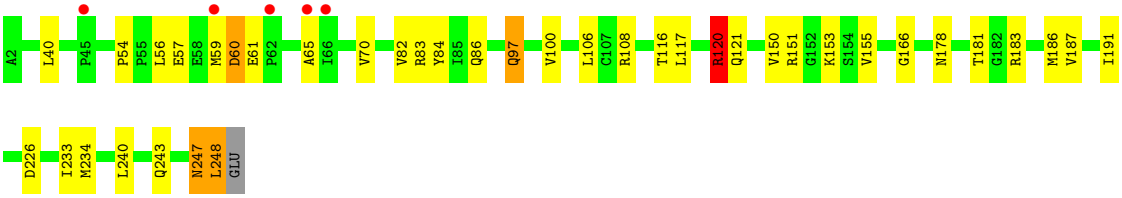
- Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	19.93 – 1.80 19.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.93-1.80) 98.2 (19.93-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.195 0.150 , 0.195	Depositor DCC
R_{free} test set	10625 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.010 for -h,-l,-k 0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21893	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, XP8, TP7, MGN, F43, MG, GL3, ACT, SMC, AGM, MHS, COM, EDO

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	1.59	20/4492 (0.4%)	1.19	9/6099 (0.1%)
1	D	1.65	31/4459 (0.7%)	1.25	6/6052 (0.1%)
2	B	1.59	14/3527 (0.4%)	1.24	9/4770 (0.2%)
2	E	1.51	13/3524 (0.4%)	1.20	8/4766 (0.2%)
3	C	1.45	7/2111 (0.3%)	1.22	2/2841 (0.1%)
3	F	1.42	9/2120 (0.4%)	1.21	5/2854 (0.2%)
All	All	1.56	94/20233 (0.5%)	1.22	39/27382 (0.1%)

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	ALA	N-CA	7.87	1.55	1.46
3	C	191	ILE	CA-CB	7.24	1.64	1.54
1	A	467	PRO	C-O	6.98	1.32	1.23
1	A	182	ILE	CA-CB	6.90	1.61	1.53
2	E	423	ASP	C-O	-6.72	1.16	1.24
2	B	159	ALA	CA-CB	6.66	1.64	1.53
2	E	200	VAL	N-CA	6.56	1.54	1.46
3	C	155	VAL	CA-CB	6.47	1.63	1.54
3	F	155	VAL	CA-CB	6.46	1.62	1.54
1	D	214	VAL	CA-CB	6.45	1.63	1.54
1	D	334	ALA	C-O	6.43	1.31	1.24
2	E	130	ALA	N-CA	6.40	1.51	1.46
1	D	540	ALA	CA-CB	6.37	1.62	1.53
2	B	220	GLN	N-CA	6.34	1.54	1.46
1	A	181	VAL	CA-CB	6.30	1.61	1.54
2	E	202	ALA	CA-CB	6.30	1.63	1.53
1	A	310	THR	N-CA	6.27	1.53	1.46
3	F	57	GLU	N-CA	6.24	1.53	1.46
1	D	495	PRO	N-CA	6.24	1.55	1.47
2	E	204	THR	C-O	6.17	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	ILE	CA-CB	-6.14	1.47	1.54
1	D	494	ALA	CA-CB	-6.13	1.43	1.53
2	B	207	ASN	CA-C	6.13	1.60	1.52
1	D	237	SER	C-O	6.04	1.31	1.24
1	D	378	THR	N-CA	5.95	1.53	1.46
1	D	42[A]	ASN	C-O	5.91	1.30	1.24
1	D	42[B]	ASN	C-O	5.91	1.30	1.24
1	D	514	ALA	CA-CB	5.88	1.60	1.52
3	C	157	GLY	N-CA	5.84	1.53	1.45
2	B	89	ALA	N-CA	5.84	1.53	1.46
1	A	292	SER	C-O	5.78	1.30	1.24
1	A	255	ALA	CA-CB	5.76	1.62	1.53
2	E	194	ASN	CA-CB	5.76	1.60	1.52
1	D	235	MET	C-O	5.75	1.30	1.24
1	D	219	ASP	CA-C	5.74	1.59	1.52
1	D	321	GLY	N-CA	5.72	1.52	1.45
2	E	415	ILE	C-O	-5.67	1.17	1.24
1	A	68	VAL	CA-C	5.66	1.58	1.52
1	A	289	ILE	CA-CB	5.64	1.61	1.54
1	A	7	ILE	CA-CB	5.55	1.60	1.54
1	D	533	ALA	N-CA	5.54	1.53	1.46
3	F	54	PRO	CA-C	5.54	1.57	1.52
2	E	370	GLY	N-CA	5.52	1.53	1.45
1	D	223	THR	N-CA	5.51	1.52	1.46
2	B	185	LEU	N-CA	5.50	1.53	1.46
1	A	281	VAL	N-CA	5.49	1.50	1.46
2	B	395	ALA	CA-CB	-5.49	1.44	1.53
1	A	264	GLY	N-CA	5.48	1.51	1.45
1	A	184	ILE	CA-C	5.47	1.59	1.52
2	B	282	ILE	C-O	5.45	1.29	1.23
2	E	139	VAL	CA-CB	5.45	1.60	1.54
1	A	472	GLY	N-CA	5.45	1.52	1.44
3	C	150	VAL	N-CA	5.43	1.52	1.46
1	D	252	ALA	CA-CB	5.41	1.61	1.53
1	D	235	MET	N-CA	5.37	1.52	1.46
2	E	141	ALA	N-CA	5.35	1.52	1.46
1	D	254	ALA	CA-C	5.35	1.59	1.52
3	C	80	ASP	N-CA	5.34	1.52	1.46
1	A	65	GLY	N-CA	5.33	1.52	1.45
1	A	494	ALA	CA-C	5.31	1.58	1.52
1	D	281	VAL	N-CA	5.29	1.50	1.46
1	A	44	GLY	N-CA	5.28	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	412	SER	CA-C	5.28	1.59	1.52
2	E	265	VAL	CA-CB	5.28	1.60	1.54
3	F	70	VAL	CA-CB	5.28	1.60	1.53
1	D	411	CYS	CA-C	5.27	1.59	1.52
3	F	100	VAL	CA-C	5.26	1.59	1.52
1	D	159	ALA	CA-CB	5.25	1.62	1.53
1	D	253	TYR	CA-C	5.22	1.59	1.52
3	F	65	ALA	CA-CB	-5.21	1.45	1.53
2	B	153	ALA	CA-C	5.20	1.59	1.52
2	E	422	VAL	C-O	5.19	1.29	1.23
1	A	142	GLY	N-CA	5.18	1.52	1.45
3	F	116	THR	CA-CB	5.17	1.61	1.53
1	D	210	ILE	CA-CB	5.17	1.60	1.54
1	D	9	ALA	CA-CB	5.16	1.61	1.53
2	E	366	ILE	CA-C	5.15	1.58	1.52
3	C	114	ALA	CA-CB	5.15	1.61	1.53
1	A	530	ALA	CA-CB	5.14	1.61	1.53
3	C	126	ARG	N-CA	5.14	1.52	1.46
3	F	120	ARG	N-CA	5.14	1.52	1.46
1	A	9	ALA	CA-CB	5.13	1.61	1.53
1	D	405	VAL	C-O	5.12	1.29	1.24
3	F	226	ASP	N-CA	5.12	1.52	1.46
2	B	204	THR	N-CA	5.10	1.52	1.46
2	B	139	VAL	CA-CB	5.09	1.60	1.54
1	D	424	LEU	N-CA	5.08	1.52	1.46
2	B	308	ALA	CA-CB	5.07	1.61	1.53
1	D	454	ALA	N-CA	5.07	1.52	1.46
1	D	246	ALA	CA-CB	5.07	1.61	1.53
1	A	501	ASP	N-CA	5.05	1.52	1.46
2	B	417	GLU	N-CA	5.04	1.52	1.46
1	D	440	ARG	N-CA	5.04	1.52	1.46
1	D	181	VAL	CA-CB	5.02	1.60	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	108	ARG	N-CA-C	7.14	122.25	112.90
1	A	280	GLY	CA-C-N	-6.77	117.72	122.59
1	A	280	GLY	C-N-CA	-6.77	117.72	122.59
2	B	187	GLY	CA-C-N	-6.70	112.88	119.78
2	B	187	GLY	C-N-CA	-6.70	112.88	119.78
2	E	18	VAL	N-CA-C	-6.42	106.73	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	481	ASN	N-CA-C	6.28	119.70	109.59
2	E	211	ALA	N-CA-C	-6.27	104.52	111.36
1	A	450	ASP	N-CA-CB	6.26	120.78	110.39
2	E	21	GLN	N-CA-C	6.11	119.99	111.74
2	B	18	VAL	N-CA-C	-6.07	106.82	111.62
1	D	450	ASP	N-CA-CB	6.06	120.45	110.39
2	B	98	ASP	N-CA-C	6.02	120.20	112.86
3	F	233	ILE	N-CA-C	-5.89	104.77	110.72
3	C	73	ILE	N-CA-C	-5.82	103.63	110.21
1	A	269	VAL	N-CA-C	5.76	116.49	110.62
3	F	40	LEU	N-CA-C	5.67	117.92	111.11
2	B	201	VAL	N-CA-C	-5.67	105.00	110.72
2	B	410	ALA	N-CA-C	5.66	117.44	111.28
2	E	385	SER	N-CA-C	-5.63	101.31	110.20
2	E	53	ILE	N-CA-C	-5.60	105.27	110.53
2	B	333	TYR	CA-CB-CG	-5.58	103.86	113.90
1	A	128	THR	N-CA-C	-5.50	105.44	111.82
2	E	178	MET	N-CA-C	-5.43	106.50	113.23
2	E	439	ILE	N-CA-C	5.42	118.19	112.83
2	B	288	LEU	N-CA-C	-5.28	101.62	109.96
1	A	354	VAL	N-CA-C	5.28	115.49	110.42
1	D	231	ILE	N-CA-C	-5.26	105.26	110.62
1	A	460	ILE	N-CA-C	5.24	117.15	112.17
2	E	79	VAL	N-CA-C	-5.20	105.47	110.72
1	D	240	LYS	N-CA-C	5.15	118.73	111.52
3	C	208	GLU	N-CA-C	5.12	116.86	111.28
1	A	333	TYR	N-CA-C	-5.10	105.85	111.71
2	B	371	GLY	CA-C-O	-5.10	117.52	122.46
3	F	97	GLN	N-CA-C	-5.06	102.32	108.14
1	D	391	LEU	N-CA-C	-5.05	105.85	111.36
3	F	187	VAL	CB-CA-C	-5.03	104.56	110.84
1	A	128	THR	N-CA-CB	5.02	118.06	110.28
1	D	411	CYS	N-CA-C	-5.02	105.81	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4408	0	4186	31	0
1	D	4359	0	4196	41	0
2	B	3422	0	3450	38	0
2	E	3431	0	3455	24	0
3	C	2059	0	1985	21	0
3	F	2071	0	2003	28	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	2	0
5	D	62	0	43	3	0
6	A	21	0	19	3	0
6	D	21	0	19	1	0
7	A	7	0	5	1	0
7	D	7	0	5	0	0
8	A	22	0	21	1	0
8	D	22	0	21	1	0
9	A	4	0	3	0	0
10	A	8	0	12	0	0
10	D	8	0	12	3	0
11	D	1	0	0	0	0
12	A	435	0	0	3	0
12	B	349	0	0	4	0
12	C	201	0	0	3	0
12	D	421	0	0	8	0
12	E	314	0	0	3	0
12	F	173	0	0	4	0
All	All	21893	0	19478	158	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 (158) 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)
1:D:432:TYR:CB	3:F:234[B]:MET:HE3	1.70	1.22
2:B:196[A]:MET:CE	2:B:198:ASN:HB2	1.71	1.18
2:B:196[A]:MET:HE3	2:B:198:ASN:HB2	1.04	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:TYR:HB2	3:F:234[B]:MET:HE3	1.37	1.04
1:D:432:TYR:HB3	3:F:234[B]:MET:HE3	1.37	1.03
2:B:196[A]:MET:HE3	2:B:198:ASN:CB	1.88	1.02
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:HH11	1.40	0.87
1:D:432:TYR:HB2	3:F:234[B]:MET:CE	2.07	0.85
1:D:432:TYR:CB	3:F:234[B]:MET:CE	2.58	0.77
1:D:433:LEU:HD23	3:F:234[B]:MET:SD	2.26	0.76
2:B:196[A]:MET:CE	2:B:198:ASN:CB	2.58	0.73
1:D:42[A]:ASN:ND2	12:D:1802:HOH:O	2.21	0.73
2:B:188:PRO:HD3	12:E:1304:HOH:O	1.89	0.73
3:F:183[B]:ARG:NH1	12:F:4120:HOH:O	2.21	0.71
1:D:433:LEU:CD2	3:F:234[B]:MET:SD	2.82	0.67
1:A:17[B]:SER:OG	1:A:20:GLU:HG3	1.96	0.65
1:D:429:LEU:HD12	3:F:234[B]:MET:HE1	1.82	0.61
1:A:194[B]:GLU:HG2	12:A:2095:HOH:O	2.00	0.61
3:F:56:LEU:HA	3:F:59:MET:HG3	1.82	0.61
2:B:196[A]:MET:HE1	2:B:198:ASN:HB2	1.78	0.60
3:C:56:LEU:O	3:C:59[A]:MET:HB2	2.01	0.60
1:D:348:TYR:CZ	10:D:555:EDO:H11	2.37	0.59
1:D:383[B]:GLU:HG2	1:D:387[B]:GLU:OE2	2.03	0.59
3:F:56:LEU:O	3:F:59:MET:HB2	2.01	0.59
2:B:261[A]:LYS:HG3	2:B:262:GLU:HG3	1.85	0.58
1:A:241[B]:GLN:HG3	1:A:242:ALA:O	2.03	0.58
3:F:183[B]:ARG:HB2	12:F:3972[B]:HOH:O	2.03	0.58
1:A:328:VAL:HB	5:D:551:F43:H9A1	1.86	0.57
2:B:322[B]:ARG:NH1	3:C:67[B]:ARG:HG2	2.19	0.57
3:F:178[B]:ASN:HB3	3:F:181[B]:THR:OG1	2.05	0.57
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.40	0.57
2:B:405:MET:HG3	1:D:115:VAL:HG22	1.87	0.56
2:B:236[A]:MET:HE1	12:B:519:HOH:O	2.06	0.56
2:E:186:GLU:HG3	2:E:378:ASN:O	2.06	0.56
2:B:214:LEU:HB2	2:B:428:PRO:HG3	1.89	0.55
2:B:113:LEU:C	2:B:113:LEU:HD13	2.31	0.55
3:F:117:LEU:HD22	3:F:120:ARG:HD3	1.88	0.55
1:A:60:ILE:HD12	12:D:3878:HOH:O	2.06	0.55
1:D:42[A]:ASN:CG	12:D:2513:HOH:O	2.49	0.54
2:B:202:ALA:HB1	2:B:416:LYS:HB2	1.90	0.54
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.89	0.54
3:F:247:ASN:O	3:F:248:LEU:HB2	2.08	0.54
2:B:68[A]:LYS:HE3	12:B:1528:HOH:O	2.08	0.53
1:D:191:ASP:HB2	12:D:3703:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD12	1:A:273:ARG:HB2	1.90	0.53
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:NH1	2.14	0.53
2:B:126:GLU:HB3	2:E:126:GLU:HB3	1.91	0.53
1:D:46[B]:GLU:HG3	12:D:693:HOH:O	2.09	0.53
2:E:206:LYS:NZ	2:E:409:GLU:OE2	2.35	0.52
2:E:429:LEU:O	2:E:433:VAL:HG23	2.10	0.52
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.40	0.52
3:F:86:GLN:HG2	3:F:151:ARG:O	2.09	0.51
3:C:65:ALA:O	3:C:69:MET:HG3	2.10	0.51
1:A:105[B]:VAL:HG13	1:A:223:THR:HG22	1.91	0.51
2:B:196[A]:MET:HE3	2:B:198:ASN:CA	2.39	0.51
1:A:4[A]:LYS:NZ	12:A:2253:HOH:O	2.33	0.51
2:E:61[A]:LYS:HG2	2:E:68[A]:LYS:HB2	1.93	0.50
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.93	0.50
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CG	2.20	0.50
3:F:82:VAL:O	3:F:83:ARG:HD2	2.11	0.50
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.47	0.50
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.47	0.50
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.47	0.50
3:C:34:GLU:HB2	12:C:1830:HOH:O	2.12	0.50
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.94	0.49
2:B:196[A]:MET:HE1	2:B:412:SER:OG	2.12	0.49
1:A:105[B]:VAL:HG13	1:A:223:THR:CG2	2.42	0.49
1:A:176[B]:ILE:O	1:A:177[B]:ASP:C	2.56	0.49
2:E:61[B]:LYS:HE3	12:E:2370:HOH:O	2.13	0.49
3:C:62:PRO:O	3:C:67[A]:ARG:NH2	2.43	0.48
3:F:153:LYS:NZ	12:F:1186:HOH:O	2.34	0.48
2:B:246[B]:MET:HE1	2:B:432:VAL:HG12	1.94	0.48
1:D:42[A]:ASN:ND2	12:D:2513:HOH:O	2.45	0.48
1:A:242:ALA:HB2	3:F:84:TYR:CZ	2.48	0.48
2:B:322[A]:ARG:HH12	3:C:61:GLU:CD	2.21	0.48
2:B:130:ALA:HB3	2:B:131:PRO:CD	2.45	0.47
1:D:451:GLN:HB2	2:E:354:GLY:CA	2.45	0.47
1:A:445:GL3:HA2	2:B:357:VAL:HG12	1.96	0.47
3:C:67[B]:ARG:NH1	12:C:3948:HOH:O	2.38	0.47
1:A:444:TYR:CE1	2:B:360:SER:HB3	2.50	0.47
3:C:45:PRO:HB3	12:C:3636:HOH:O	2.13	0.47
3:C:82:VAL:O	3:C:83:ARG:HD2	2.14	0.47
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.72	0.47
2:E:58:LYS:HE3	12:E:1433:HOH:O	2.15	0.47
1:D:358:TYR:OH	1:D:372[A]:ASP:OD2	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:243[B]:GLN:NE2	12:F:891:HOH:O	2.46	0.46
2:E:333:TYR:HB2	3:F:106:LEU:HD22	1.98	0.46
1:A:279:GLY:HA2	1:A:473:PRO:HB2	1.97	0.46
1:A:480:MET:O	6:A:552[A]:TP7:H32C	2.15	0.46
1:D:106:ILE:HB	1:D:261:ILE:HB	1.98	0.46
2:E:214:LEU:HB2	2:E:428:PRO:HG3	1.97	0.46
2:E:331:LEU:HB3	2:E:356:ALA:HB2	1.98	0.46
1:D:8:ASN:O	1:D:12[B]:LYS:HG2	2.16	0.45
2:E:374:ILE:C	2:E:374:ILE:HD12	2.42	0.45
12:B:2205:HOH:O	2:E:188:PRO:HD3	2.16	0.45
1:D:150:MET:HA	1:D:150:MET:HE2	1.99	0.45
3:F:60:ASP:O	3:F:60:ASP:CG	2.60	0.45
2:E:242:ALA:O	2:E:246[A]:MET:HB2	2.16	0.45
1:A:145:VAL:HG23	1:A:146:VAL:HG23	1.99	0.45
1:D:305:LEU:CD1	1:D:344:ASP:HA	2.47	0.45
1:D:109:LEU:HB2	1:D:204[B]:ILE:HG23	1.98	0.44
1:A:383[A]:GLU:HG3	12:A:2606:HOH:O	2.17	0.44
2:B:196[A]:MET:HB3	2:B:196[A]:MET:HE2	1.74	0.44
1:A:544:ALA:HB2	12:D:3604[A]:HOH:O	2.18	0.44
2:B:186:GLU:HG3	2:B:378:ASN:O	2.18	0.44
3:C:67[A]:ARG:HE	3:C:67[A]:ARG:HB3	1.25	0.44
2:B:233[B]:PHE:CD1	3:C:248:LEU:HD12	2.53	0.44
1:D:21:LYS:HG2	1:D:389:PRO:HG2	2.00	0.44
2:B:14[A]:ARG:HH12	3:C:63:GLU:HG2	1.83	0.44
2:B:333:TYR:HB2	3:C:106:LEU:HD22	2.01	0.43
6:A:552[A]:TP7:H42C	6:A:552[A]:TP7:H72C	1.84	0.43
1:D:12[B]:LYS:HA	1:D:12[B]:LYS:HD3	1.87	0.43
1:A:480:MET:O	8:A:554[B]:XP8:H3A	2.17	0.43
1:D:480:MET:O	8:D:553[B]:XP8:H3A	2.18	0.43
2:B:246[B]:MET:HE2	2:B:246[B]:MET:HB3	1.77	0.43
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.59	0.43
1:A:217:THR:HG23	12:D:679:HOH:O	2.19	0.43
1:D:22:LYS:NZ	10:D:554:EDO:H12	2.34	0.43
1:D:448:LEU:O	1:D:452:SMC:HCS3	2.19	0.43
2:B:322[B]:ARG:CZ	3:C:67[B]:ARG:HG2	2.49	0.42
1:D:7:ILE:CG2	1:D:11:LYS:HE3	2.48	0.42
10:D:554:EDO:H11	3:F:166:GLY:HA3	2.01	0.42
3:C:117:LEU:HD13	3:C:120:ARG:HG3	2.00	0.42
1:D:243:ALA:HB1	5:D:551:F43:H9B1	2.01	0.42
1:A:481:ASN:HA	6:A:552[A]:TP7:S7	2.59	0.42
2:B:41:GLY:C	2:B:425:PHE:HZ	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:TYR:CD1	2:B:165:PRO:HA	2.54	0.42
1:D:145:VAL:HG23	1:D:146:VAL:HG23	2.01	0.42
1:D:383[B]:GLU:CG	1:D:387[B]:GLU:OE2	2.67	0.42
1:D:439:SER:HB3	3:F:97:GLN:HB3	2.02	0.42
7:A:553:COM:H12	5:D:551:F43:C1C	2.50	0.42
3:F:191:ILE:HD12	3:F:191:ILE:HA	1.91	0.42
1:A:84:ASP:HA	1:D:151:VAL:HB	2.02	0.42
1:A:367:MET:HE2	1:A:367:MET:HB2	1.88	0.42
2:B:13:ASP:OD1	12:B:3793:HOH:O	2.22	0.42
2:B:58:LYS:HE2	2:B:58:LYS:HB3	1.55	0.42
2:B:113:LEU:HD23	2:B:418:VAL:HG13	2.01	0.42
1:D:449:GLN:CD	1:D:484:HIS:CD2	2.98	0.41
1:A:332:GLN:HA	1:A:335:THR:OG1	2.19	0.41
2:B:191:ALA:HB3	2:E:125:ALA:CB	2.49	0.41
3:C:99:TYR:CD1	3:C:116:THR:HG21	2.56	0.41
2:E:324:ALA:O	2:E:327:VAL:HG12	2.20	0.41
1:D:332:GLN:HA	1:D:335:THR:OG1	2.21	0.41
1:D:383[B]:GLU:OE2	1:D:387[B]:GLU:OE2	2.38	0.41
2:B:407:SER:HB2	2:B:408:PRO:CD	2.50	0.41
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.96	0.41
2:E:246[B]:MET:HB3	2:E:246[B]:MET:HE2	1.81	0.41
2:B:374:ILE:HD12	2:B:374:ILE:C	2.46	0.40
1:A:257:MHS:NE2	6:D:1[A]:TP7:O1P	2.55	0.40
5:A:1:F43:C9A	5:A:1:F43:CBA	2.99	0.40
2:E:3[A]:LYS:HB2	2:E:3[A]:LYS:HE3	1.76	0.40
2:E:339:GLU:HG3	2:E:346:SER:HB3	2.02	0.40
3:F:240:LEU:HD23	3:F:240:LEU:HA	1.98	0.40
2:E:288:LEU:HD23	2:E:288:LEU:HA	1.96	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	564/549 (103%)	543 (96%)	20 (4%)	1 (0%)	43	31
1	D	560/549 (102%)	543 (97%)	16 (3%)	1 (0%)	43	31
2	B	459/442 (104%)	448 (98%)	10 (2%)	1 (0%)	43	31
2	E	459/442 (104%)	449 (98%)	10 (2%)	0	100	100
3	C	254/248 (102%)	243 (96%)	11 (4%)	0	100	100
3	F	256/248 (103%)	246 (96%)	10 (4%)	0	100	100
All	All	2552/2478 (103%)	2472 (97%)	77 (3%)	3 (0%)	48	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	SER
1	A	325	SER
2	B	402	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	456/434 (105%)	453 (99%)	3 (1%)	76	73
1	D	452/434 (104%)	446 (99%)	6 (1%)	61	54
2	B	360/341 (106%)	353 (98%)	7 (2%)	50	41
2	E	360/341 (106%)	353 (98%)	7 (2%)	50	41
3	C	224/216 (104%)	218 (97%)	6 (3%)	39	27
3	F	225/216 (104%)	217 (96%)	8 (4%)	31	18
All	All	2077/1982 (105%)	2040 (98%)	37 (2%)	51	43

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	PRO
1	A	186	LYS

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Mol	Chain	Res	Type
1	A	450	ASP
2	B	3	LYS
2	B	58	LYS
2	B	65	PRO
2	B	97	GLU
2	B	113	LEU
2	B	185	LEU
2	B	283	LYS
3	C	61	GLU
3	C	67[A]	ARG
3	C	67[B]	ARG
3	C	150	VAL
3	C	186	MET
3	C	248	LEU
1	D	54	PRO
1	D	84	ASP
1	D	186	LYS
1	D	450	ASP
1	D	476	PRO
1	D	545	LEU
2	E	126	GLU
2	E	185	LEU
2	E	278	GLU
2	E	283	LYS
2	E	374	ILE
2	E	438[A]	GLU
2	E	438[B]	GLU
3	F	60	ASP
3	F	61	GLU
3	F	120	ARG
3	F	121	GLN
3	F	150	VAL
3	F	186	MET
3	F	247	ASN
3	F	248	LEU

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	73	GLN
1	A	317	GLN

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Mol	Chain	Res	Type
2	B	174	ASN
2	B	318	GLN
3	C	121	GLN
1	D	73	GLN
1	D	111	HIS
1	D	437	GLN
2	E	174	ASN
2	E	318	GLN
3	F	42	HIS
3	F	121	GLN
3	F	247	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SMC	A	452	1	5,6,7	0.95	0	3,6,8	2.20	1 (33%)
1	GL3	D	445	1	2,3,4	3.48	1 (50%)	1,2,4	1.07	0
1	AGM	A	271	1	10,11,12	1.38	2 (20%)	7,13,15	2.63	4 (57%)
1	MGN	D	400	1	6,9,10	1.67	1 (16%)	7,12,14	1.79	1 (14%)
1	GL3	A	445	1	2,3,4	3.17	1 (50%)	1,2,4	0.12	0
1	MHS	D	257	1	10,11,12	2.35	3 (30%)	5,14,16	10.16	4 (80%)
1	MHS	A	257	1	10,11,12	2.80	5 (50%)	5,14,16	10.78	4 (80%)
1	MGN	A	400	1	6,9,10	2.12	1 (16%)	7,12,14	1.74	1 (14%)
1	AGM	D	271	1	10,11,12	1.62	3 (30%)	7,13,15	2.15	4 (57%)
1	SMC	D	452	1	5,6,7	0.77	0	3,6,8	2.18	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
1	SMC	A	452	1	-	1/3/5/7	-
1	GL3	D	445	1	-	1/1/1/2	-
1	AGM	A	271	1	-	3/10/11/13	-
1	MGN	D	400	1	-	0/7/9/12	-
1	GL3	A	445	1	-	1/1/1/2	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	D	271	1	-	1/10/11/13	-
1	SMC	D	452	1	-	1/3/5/7	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	MHS	CE1-NE2	5.87	1.47	1.32
1	A	257	MHS	CE1-NE2	5.47	1.46	1.32
1	D	445	GL3	C-S	-4.90	1.60	1.80
1	A	400	MGN	CB1-CA	4.61	1.60	1.55
1	A	445	GL3	C-S	-4.44	1.62	1.80
1	A	257	MHS	CE1-ND1	4.05	1.46	1.35
1	A	257	MHS	CD2-CG	3.43	1.41	1.36
1	D	271	AGM	CG-CD	3.38	1.58	1.53
1	D	400	MGN	CB1-CA	-3.34	1.51	1.55
1	A	257	MHS	CM-ND1	3.13	1.52	1.46
1	D	257	MHS	CE1-ND1	2.54	1.42	1.35
1	A	271	AGM	CZ-NH2	2.52	1.41	1.32
1	A	257	MHS	CG-ND1	-2.25	1.34	1.38
1	D	271	AGM	CB-CA	2.21	1.56	1.53
1	D	271	AGM	O-C	2.13	1.28	1.20
1	A	271	AGM	CG-CB	2.11	1.58	1.53
1	D	257	MHS	CM-ND1	2.09	1.50	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	MHS	ND1-CE1-NE2	-22.80	99.36	112.94
1	D	257	MHS	ND1-CE1-NE2	-21.56	100.11	112.94
1	A	257	MHS	CM-ND1-CE1	-6.49	114.14	126.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	MHS	CM-ND1-CE1	-6.07	114.92	126.28
1	A	400	MGN	CB1-CG-CD	-4.26	103.62	112.13
1	A	271	AGM	NE1-CZ-NH2	-4.13	113.50	120.58
1	D	400	MGN	CB1-CG-CD	-4.00	104.15	112.13
1	A	452	SMC	CA-CB-SG	-3.74	107.99	114.04
1	A	271	AGM	CE2-CD-CG	3.70	118.24	111.48
1	D	452	SMC	CA-CB-SG	-3.66	108.11	114.04
1	A	257	MHS	CD2-NE2-CE1	3.50	109.82	105.24
1	A	271	AGM	NH1-CZ-NE1	3.06	126.32	119.58
1	D	271	AGM	CE2-CD-CG	3.04	117.03	111.48
1	D	257	MHS	CD2-NE2-CE1	2.97	109.12	105.24
1	D	271	AGM	NH1-CZ-NE1	2.88	125.94	119.58
1	D	271	AGM	CG-CD-NE1	-2.67	105.83	110.42
1	A	257	MHS	CM-ND1-CG	2.62	129.48	126.69
1	D	257	MHS	CM-ND1-CG	2.42	129.27	126.69
1	D	271	AGM	NH1-CZ-NH2	-2.13	114.00	120.07
1	A	271	AGM	CE2-CD-NE1	-2.02	105.21	110.31

There are no chirality outliers.

All (8) 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	A	271	AGM	CE2-CD-CG-CB
1	A	271	AGM	NE1-CD-CG-CB
1	D	271	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0
1	A	257	MHS	1	0
1	D	452	SMC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	TP7	A	552[A]	-	19,20,20	1.05	1 (5%)	24,26,26	1.18	1 (4%)
6	TP7	D	1[A]	-	19,20,20	0.91	1 (5%)	24,26,26	0.98	0
5	F43	A	1	7,1	63,71,71	2.47	16 (25%)	73,118,118	1.62	13 (17%)
7	COM	D	552	5	6,6,6	2.68	2 (33%)	8,8,8	2.22	3 (37%)
9	ACT	A	555[A]	4	3,3,3	0.85	0	3,3,3	1.48	0
8	XP8	A	554[B]	-	20,21,21	0.98	1 (5%)	25,27,27	1.03	0
8	XP8	D	553[B]	-	20,21,21	0.79	0	25,27,27	0.85	1 (4%)
10	EDO	A	557	-	3,3,3	0.45	0	2,2,2	0.40	0
10	EDO	D	555	-	3,3,3	0.49	0	2,2,2	0.51	0
10	EDO	A	556	-	3,3,3	0.88	0	2,2,2	0.46	0
5	F43	D	551	7,1	63,71,71	2.43	15 (23%)	73,118,118	1.92	22 (30%)
7	COM	A	553	5	6,6,6	2.82	2 (33%)	8,8,8	2.32	2 (25%)
10	EDO	D	554	-	3,3,3	0.33	0	2,2,2	0.29	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
6	TP7	A	552[A]	-	-	3/24/24/24	-
6	TP7	D	1[A]	-	-	2/24/24/24	-
5	F43	A	1	7,1	-	9/28/185/185	-
7	COM	D	552	5	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	XP8	A	554[B]	-	-	2/25/25/25	-
8	XP8	D	553[B]	-	-	2/25/25/25	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	D	555	-	-	1/1/1/1	-
10	EDO	A	556	-	-	1/1/1/1	-
5	F43	D	551	7,1	-	10/28/185/185	-
7	COM	A	553	5	-	0/4/4/4	-
10	EDO	D	554	-	-	1/1/1/1	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	551	F43	NI-NA	9.67	2.12	1.89
5	A	1	F43	NI-NB	9.39	2.12	1.89
5	A	1	F43	NI-NA	9.32	2.11	1.89
5	D	551	F43	NI-NB	8.88	2.10	1.89
5	A	1	F43	NI-ND	7.23	2.06	1.89
7	A	553	COM	C2-S2	-5.91	1.69	1.77
5	D	551	F43	NI-ND	5.76	2.03	1.89
7	D	552	COM	C2-S2	-5.51	1.69	1.77
5	D	551	F43	CHD-C1D	4.23	1.50	1.43
5	A	1	F43	CHB-C4A	4.18	1.57	1.51
5	D	551	F43	CHB-C1B	4.06	1.56	1.53
5	A	1	F43	CHA-C4D	3.99	1.57	1.53
5	D	551	F43	CHA-C4D	-3.84	1.49	1.53
5	A	1	F43	CHC-C4B	3.77	1.49	1.39
5	D	551	F43	CHC-C4B	3.69	1.49	1.39
5	A	1	F43	C5D-C6D	3.18	1.59	1.53
5	D	551	F43	CHB-C4A	3.05	1.56	1.51
6	A	552[A]	TP7	P-O4P	3.00	1.64	1.59
8	A	554[B]	XP8	P-O4P	2.99	1.64	1.59
5	D	551	F43	C3A-C4A	2.83	1.58	1.53
5	D	551	F43	CAB-C3B	2.77	1.60	1.54
5	D	551	F43	C9C-CAC	2.60	1.56	1.50
5	A	1	F43	CHB-C1B	2.50	1.55	1.53
5	A	1	F43	CHD-C1D	2.48	1.47	1.43
7	D	552	COM	O3S-S2	2.47	1.56	1.47
5	D	551	F43	C5C-C2C	2.46	1.57	1.53
5	A	1	F43	CAA-C3A	2.46	1.57	1.53
5	A	1	F43	C5C-C6C	2.44	1.57	1.51
7	A	553	COM	O2S-S2	2.37	1.51	1.45
5	A	1	F43	C3D-C4D	-2.35	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1[A]	TP7	P-O1P	2.33	1.57	1.50
5	A	1	F43	CHA-C1A	2.30	1.55	1.50
5	D	551	F43	C2A-C3A	2.22	1.58	1.54
5	A	1	F43	C4D-ND	2.19	1.52	1.49
5	A	1	F43	ODA-CCA	-2.17	1.23	1.30
5	D	551	F43	OCD-CAD	-2.15	1.23	1.30
5	A	1	F43	C9A-C2A	-2.07	1.51	1.54
5	D	551	F43	ODA-CCA	-2.05	1.24	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	551	F43	C5D-C2D-C1D	5.92	118.15	110.43
7	A	553	COM	O1S-S2-C2	5.71	115.35	106.73
5	D	551	F43	O8D-C7D-C6D	-4.16	114.05	120.87
5	D	551	F43	C2C-C5C-C6C	-4.05	106.38	113.95
5	D	551	F43	C6D-C7D-CHD	3.91	124.16	116.94
5	A	1	F43	C2B-C1B-NB	3.82	107.53	101.86
7	D	552	COM	O2S-S2-C2	3.74	112.38	106.73
7	D	552	COM	O1S-S2-C2	3.71	112.33	106.73
5	A	1	F43	OBC-CAC-C9C	3.65	125.53	114.00
5	A	1	F43	C2C-C5C-C6C	-3.57	107.26	113.95
5	D	551	F43	C2B-C1B-NB	3.42	106.94	101.86
5	D	551	F43	CAB-C3B-C2B	-3.28	111.76	119.00
5	A	1	F43	CAB-C3B-C2B	-3.27	111.78	119.00
5	D	551	F43	C1D-CHD-C4C	-3.22	116.23	125.28
5	D	551	F43	C9A-C2A-C3A	3.18	117.56	112.99
5	D	551	F43	OBC-CAC-C9C	3.11	123.84	114.00
5	D	551	F43	CHA-C4D-C3D	-3.08	109.21	117.90
5	A	1	F43	C3A-C2A-C1A	-3.07	96.91	99.97
5	D	551	F43	C4B-CHC-C1C	3.04	130.76	125.84
5	D	551	F43	C5C-C2C-C3C	-3.02	107.58	115.05
5	A	1	F43	OCC-CAC-C9C	-2.97	113.66	123.09
7	A	553	COM	O3S-S2-O2S	-2.97	103.96	111.40
5	A	1	F43	ODB-CCB-CBB	-2.90	113.89	123.09
5	A	1	F43	C9B-C2B-C8B	-2.89	103.33	110.61
6	A	552[A]	TP7	C5-C6-C7	-2.89	107.95	113.09
5	D	551	F43	C7D-CHD-C4C	2.71	127.43	121.76
5	A	1	F43	C4B-CHC-C1C	2.69	130.19	125.84
7	D	552	COM	O3S-S2-O2S	-2.66	104.75	111.40
5	D	551	F43	C1B-C2B-C3B	2.65	105.36	101.51
5	A	1	F43	O8D-C7D-C6D	-2.57	116.66	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	F43	O7B-C6B-C8B	-2.53	121.83	126.92
5	D	551	F43	C9D-C3D-C4D	-2.47	108.15	114.63
5	A	1	F43	C9A-C2A-C5A	2.44	114.88	110.74
5	D	551	F43	C9C-C8C-C3C	-2.41	106.61	113.79
5	A	1	F43	ODA-CCA-CBA	2.32	121.33	114.00
5	D	551	F43	ODB-CCB-CBB	-2.29	115.83	123.09
5	D	551	F43	CHC-C1C-NC	2.25	128.02	124.39
5	D	551	F43	C5D-C2D-C3D	-2.15	114.34	118.26
5	D	551	F43	OCC-CAC-C9C	-2.14	116.29	123.09
5	D	551	F43	C2D-C1D-CHD	-2.14	119.20	121.85
8	D	553[B]	XP8	O2P-P-O1P	2.05	115.50	107.80
5	D	551	F43	OEB-CCB-ODB	2.01	128.49	123.33

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	552	COM	C1-C2-S2-O2S
8	D	553[B]	XP8	C6-C7-C8-S8
5	D	551	F43	C3A-CAA-CBA-CCA
5	A	1	F43	C3A-CAA-CBA-CCA
10	D	554	EDO	O1-C1-C2-O2
10	D	555	EDO	O1-C1-C2-O2
6	D	1[A]	TP7	C2-C3-C4-C5
8	A	554[B]	XP8	C6-C7-C8-S8
10	A	556	EDO	O1-C1-C2-O2
6	A	552[A]	TP7	C2-C3-C4-C5
8	D	553[B]	XP8	C2-C3-C4-C5
5	A	1	F43	C2C-C5C-C6C-O8C
10	A	557	EDO	O1-C1-C2-O2
6	A	552[A]	TP7	CB-O4P-P-O3P
6	D	1[A]	TP7	CB-O4P-P-O3P
8	A	554[B]	XP8	C2-C3-C4-C5
5	A	1	F43	CAA-CBA-CCA-OEA
5	D	551	F43	CAA-CBA-CCA-ODA
5	D	551	F43	CAA-CBA-CCA-OEA
5	A	1	F43	CAA-CBA-CCA-ODA
5	A	1	F43	CAB-CBB-CCB-OEB
6	A	552[A]	TP7	C4-C5-C6-C7
5	A	1	F43	C8C-C9C-CAC-OCC
5	D	551	F43	CAB-CBB-CCB-OEB
5	D	551	F43	C3D-C9D-CAD-OBD

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Mol	Chain	Res	Type	Atoms
5	D	551	F43	C3D-C9D-CAD-OCD
5	A	1	F43	C8C-C9C-CAC-OBC
5	A	1	F43	CAB-CBB-CCB-ODB
5	A	1	F43	C2C-C5C-C6C-O7C
5	D	551	F43	C2C-C5C-C6C-O7C
5	D	551	F43	C8C-C9C-CAC-OBC
5	D	551	F43	C2C-C5C-C6C-O8C
5	D	551	F43	CAB-CBB-CCB-ODB

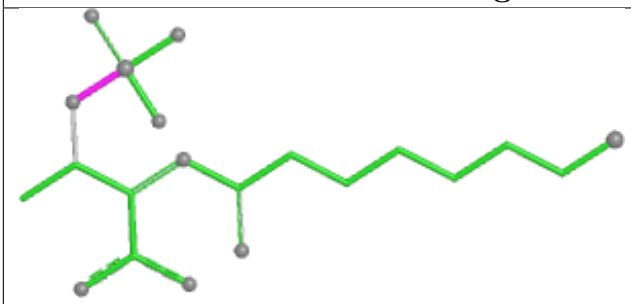
There are no ring outliers.

9 monomers are involved in 14 short contacts:

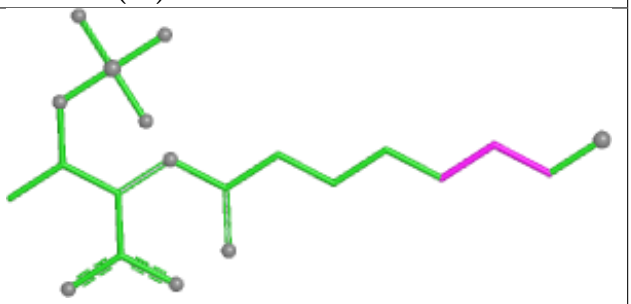
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	552[A]	TP7	3	0
6	D	1[A]	TP7	1	0
5	A	1	F43	2	0
8	A	554[B]	XP8	1	0
8	D	553[B]	XP8	1	0
10	D	555	EDO	1	0
5	D	551	F43	3	0
7	A	553	COM	1	0
10	D	554	EDO	2	0

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

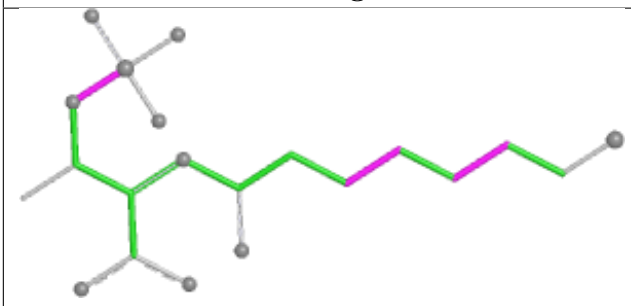
Ligand TP7 A 552 (A)



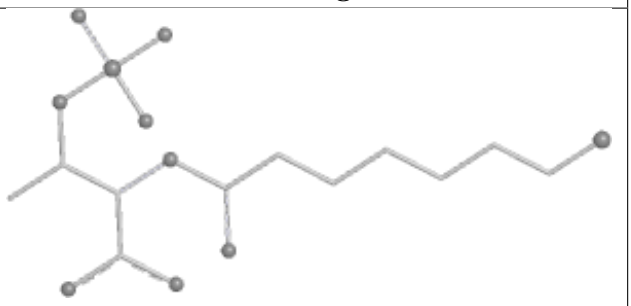
Bond lengths



Bond angles

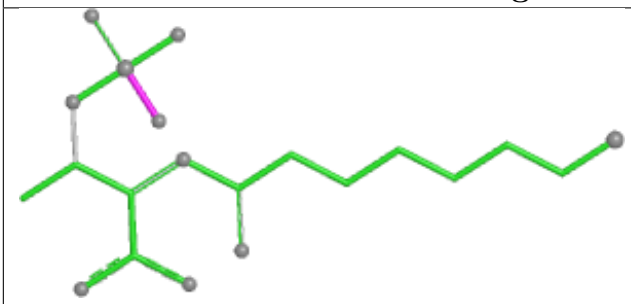


Torsions

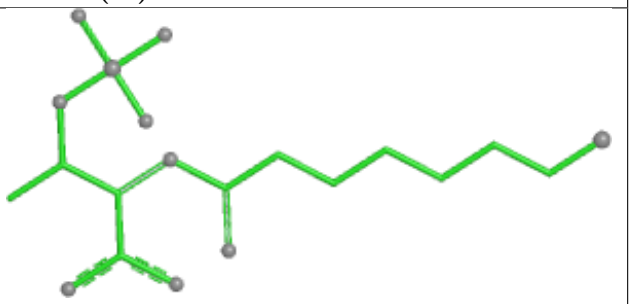


Rings

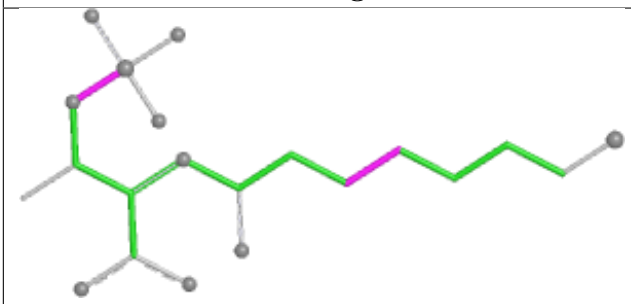
Ligand TP7 D 1 (A)



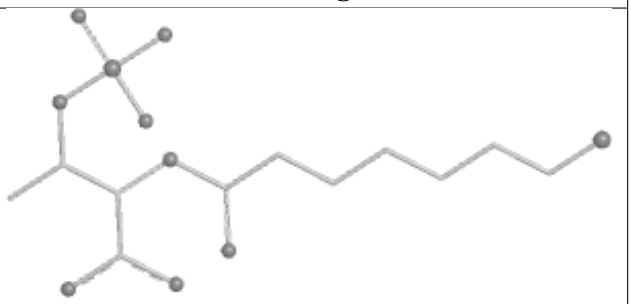
Bond lengths



Bond angles

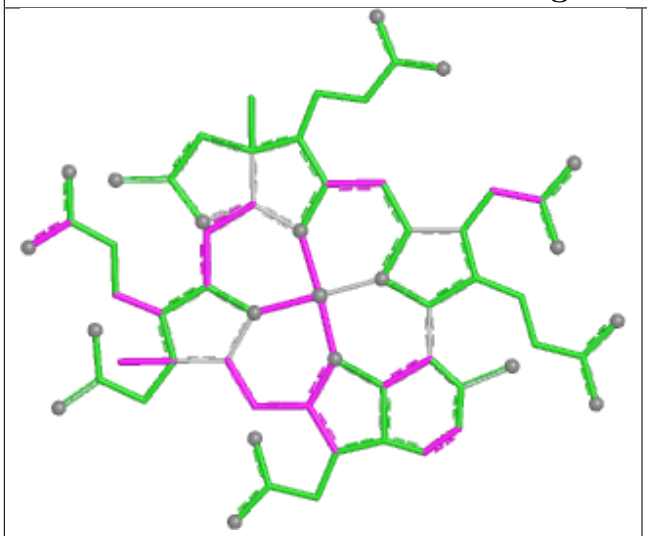


Torsions

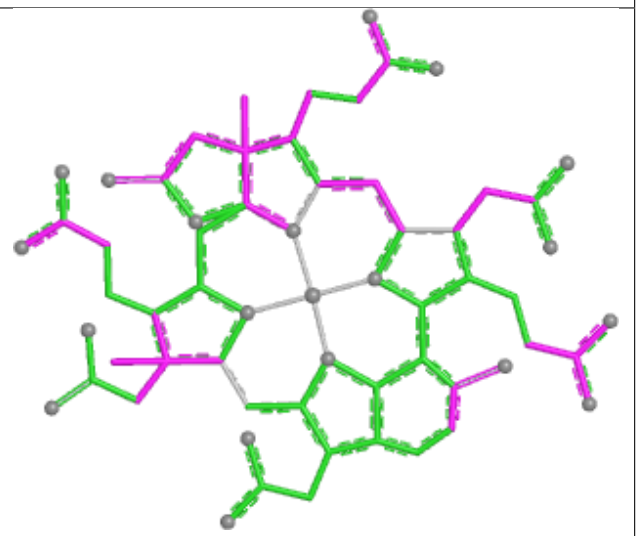


Rings

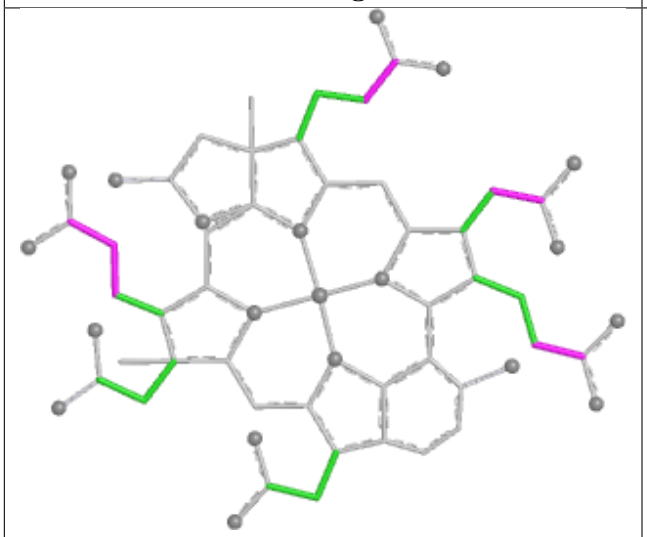
Ligand F43 A 1



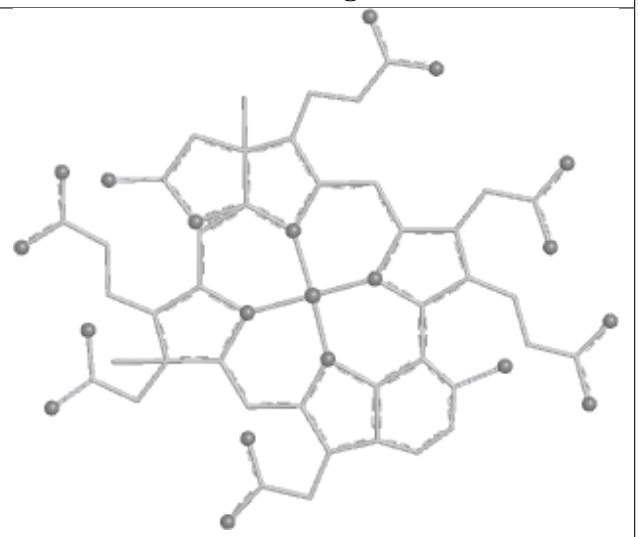
Bond lengths



Bond angles

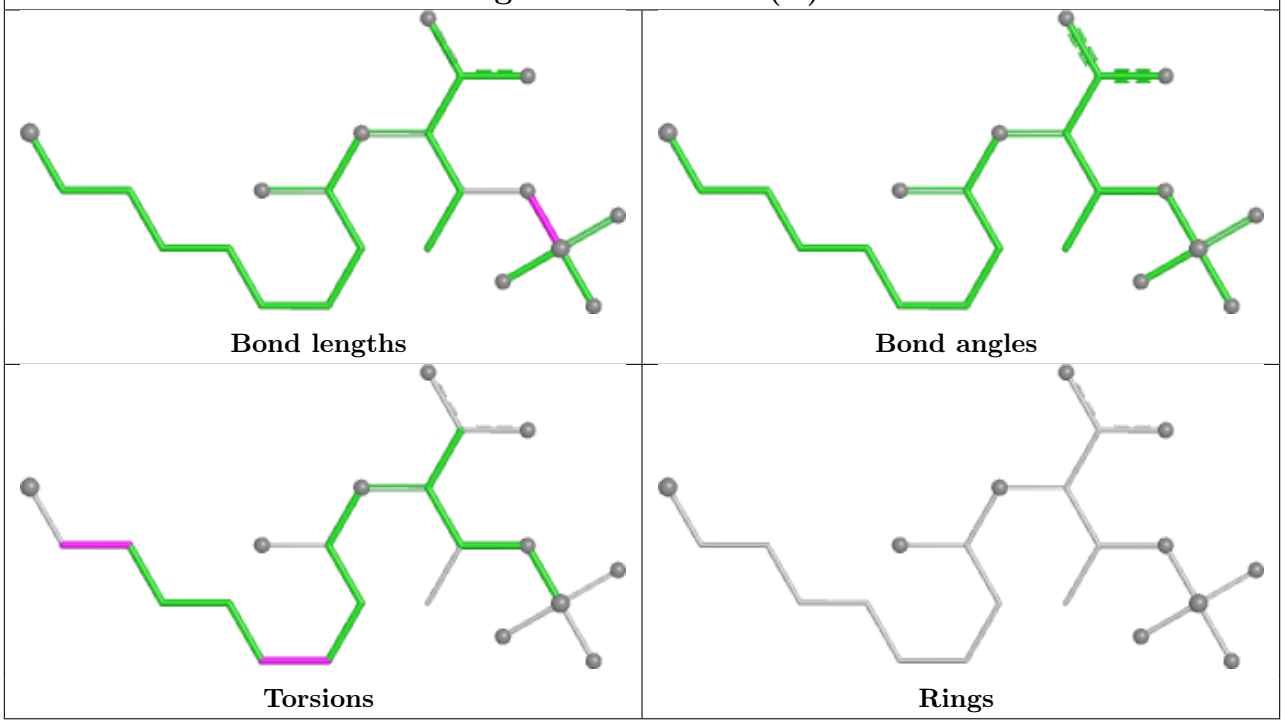


Torsions

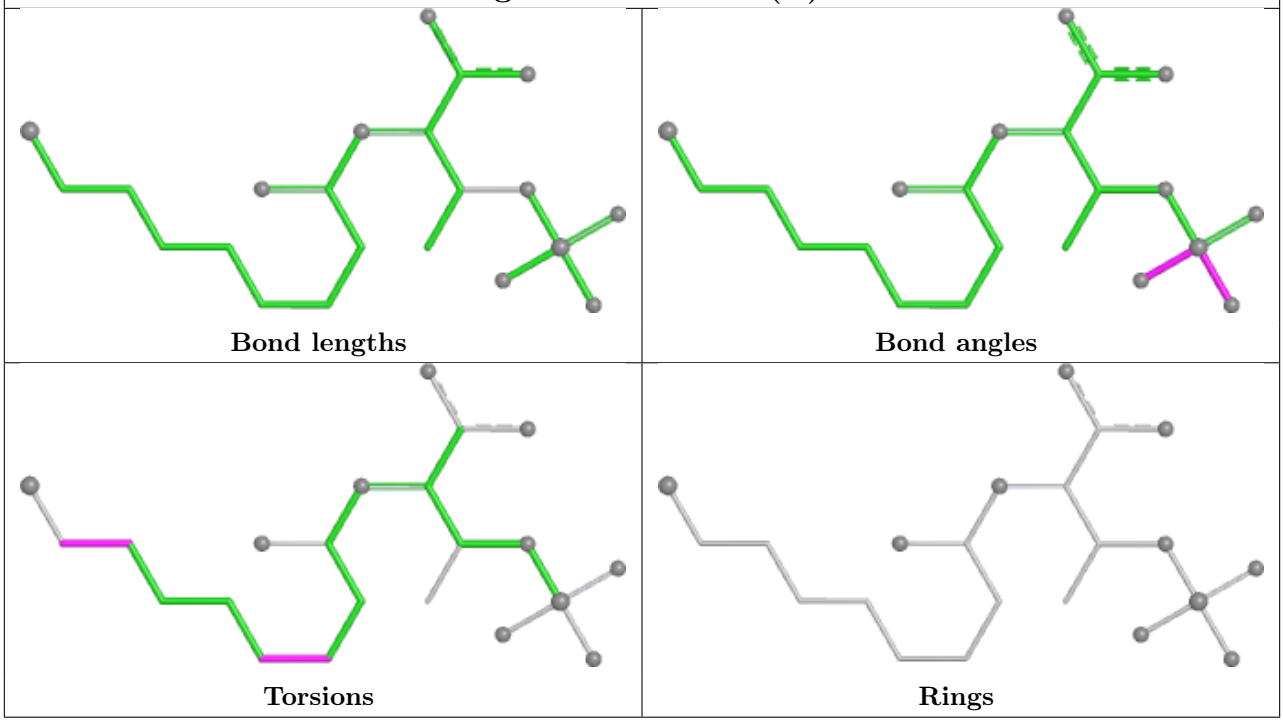


Rings

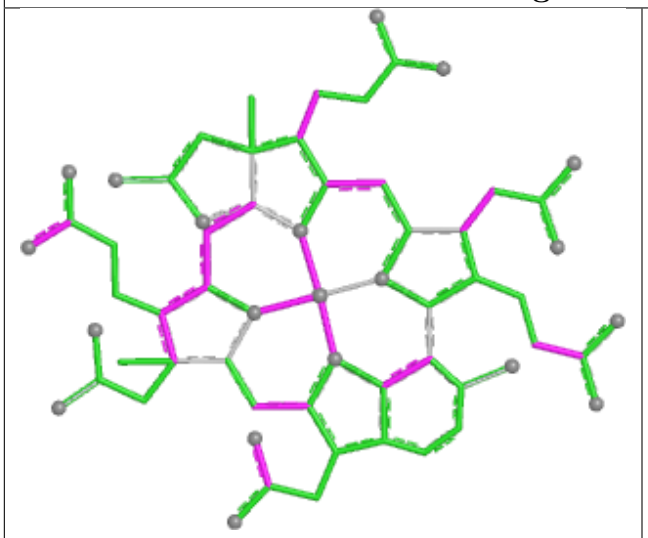
Ligand XP8 A 554 (B)



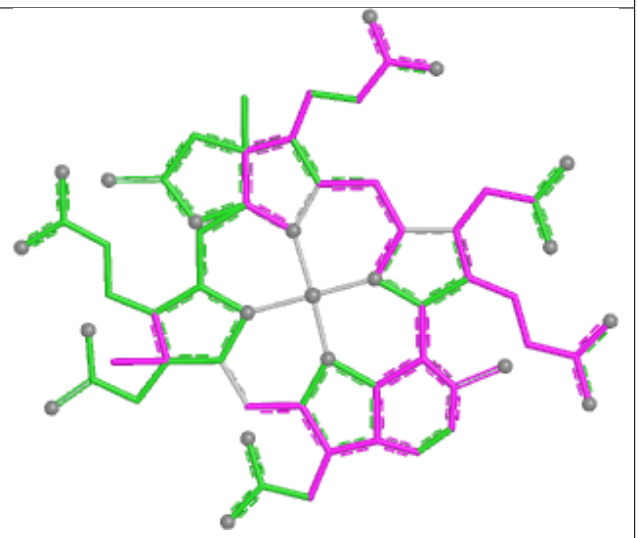
Ligand XP8 D 553 (B)



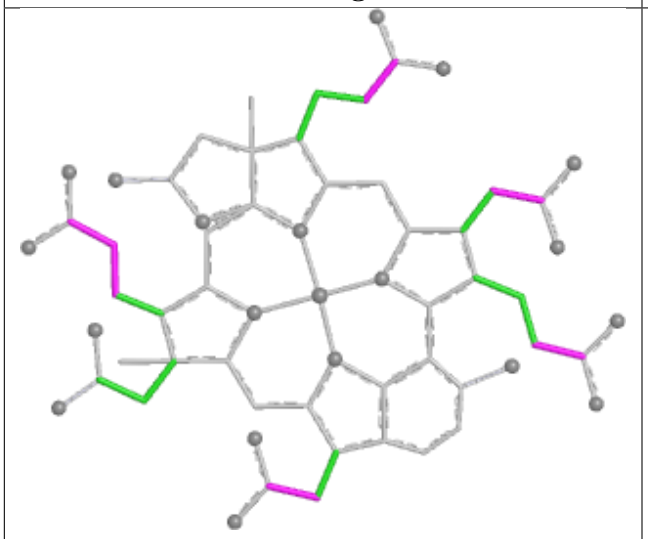
Ligand F43 D 551



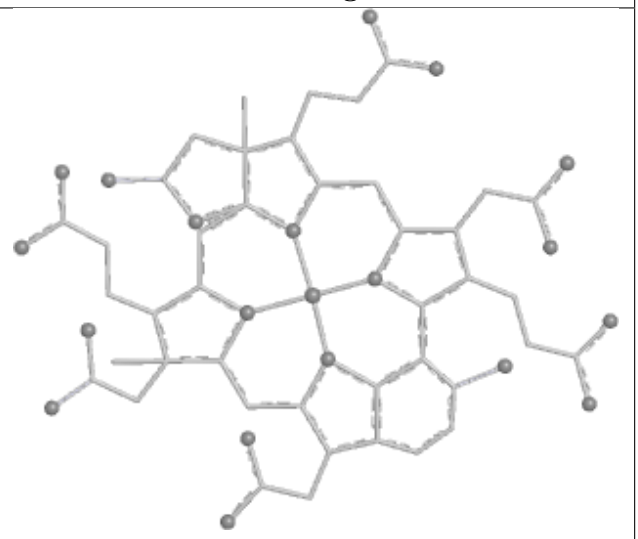
Bond lengths



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%)	-0.90	0	100	100	4, 11, 24, 39	22 (4%)
1	D	543/549 (98%)	-0.87	0	100	100	3, 11, 24, 40	19 (3%)
2	B	442/442 (100%)	-0.58	0	100	100	5, 16, 27, 43	18 (4%)
2	E	442/442 (100%)	-0.32	4 (0%)	81	81	6, 19, 36, 53	19 (4%)
3	C	248/248 (100%)	-0.48	1 (0%)	88	89	7, 18, 34, 58	8 (3%)
3	F	247/248 (99%)	-0.19	5 (2%)	65	65	8, 22, 41, 63	11 (4%)
All	All	2465/2478 (99%)	-0.62	10 (0%)	88	89	3, 15, 31, 63	97 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	62	PRO	3.2
3	F	59	MET	2.7
3	F	45	PRO	2.7
3	C	45	PRO	2.6
2	E	97	GLU	2.5
2	E	17	LEU	2.5
3	F	66	ILE	2.4
3	F	65	ALA	2.3
2	E	98	ASP	2.3
2	E	2	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MHS	A	257	11/12	0.95	0.06	15,18,21,22	0
1	MHS	D	257	11/12	0.95	0.06	15,18,20,21	0
1	AGM	D	271	12/13	0.97	0.04	7,9,11,13	0
1	SMC	A	452	7/8	0.98	0.05	7,8,11,12	0
1	AGM	A	271	12/13	0.98	0.04	7,9,10,11	0
1	MGN	A	400	10/11	0.98	0.03	6,6,11,11	0
1	MGN	D	400	10/11	0.98	0.03	7,9,10,12	0
1	SMC	D	452	7/8	0.99	0.04	9,10,13,16	0
1	GL3	D	445	4/5	1.00	0.02	7,8,9,10	0
1	GL3	A	445	4/5	1.00	0.02	6,6,7,10	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

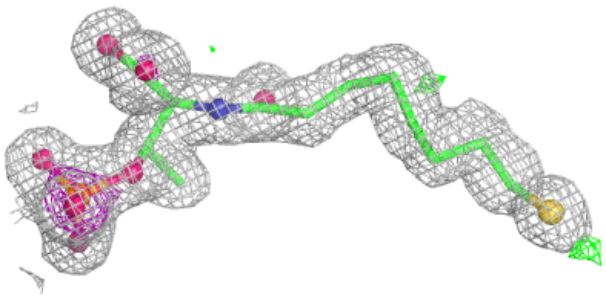
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

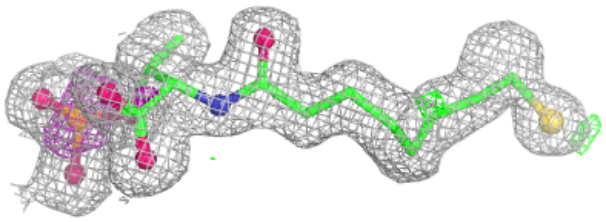
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	D	555	4/4	0.84	0.12	39,43,43,45	0
4	MG	B	444	1/1	0.87	0.08	30,30,30,30	1
10	EDO	A	556	4/4	0.89	0.11	31,31,31,34	0
10	EDO	D	554	4/4	0.91	0.11	33,38,38,38	0
10	EDO	A	557	4/4	0.91	0.12	40,42,43,44	0
4	MG	B	1	1/1	0.93	0.05	41,41,41,41	0
4	MG	A	551	1/1	0.93	0.07	22,22,22,22	1
8	XP8	D	553[B]	22/22	0.94	0.07	12,14,17,19	22
9	ACT	A	555[A]	4/4	0.94	0.07	21,21,21,22	4
8	XP8	A	554[B]	22/22	0.94	0.06	11,14,18,18	22
6	TP7	D	1[A]	21/21	0.96	0.06	12,14,17,19	21
4	MG	C	250	1/1	0.96	0.06	32,32,32,32	0
4	MG	F	250	1/1	0.96	0.05	28,28,28,28	0
6	TP7	A	552[A]	21/21	0.96	0.06	10,14,16,17	21
7	COM	D	552	7/7	0.98	0.06	14,16,18,22	0
7	COM	A	553	7/7	0.99	0.04	12,15,17,20	0
5	F43	A	1	62/62	0.99	0.03	5,9,14,19	0
5	F43	D	551	62/62	0.99	0.03	3,8,12,16	0
11	ZN	D	556	1/1	1.00	0.01	14,14,14,14	1

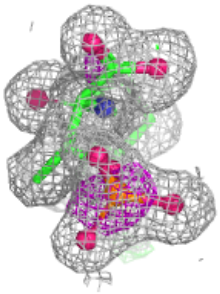
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XP8 D 553 (B):

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

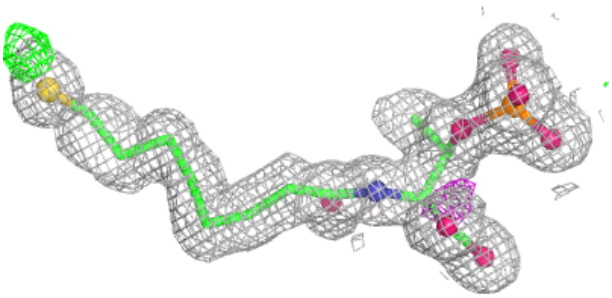


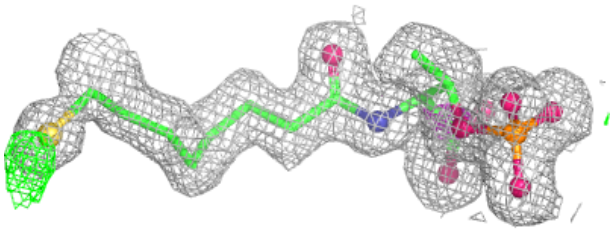


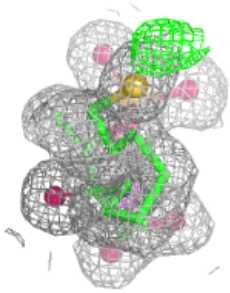


Electron density around XP8 A 554 (B):

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

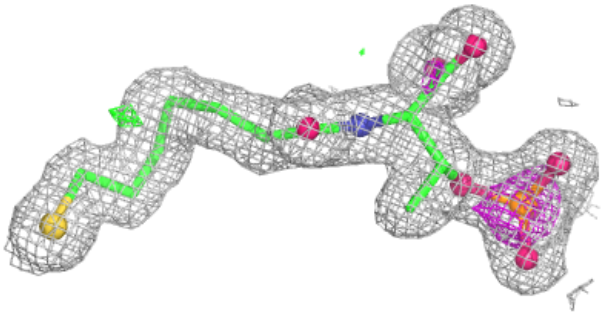


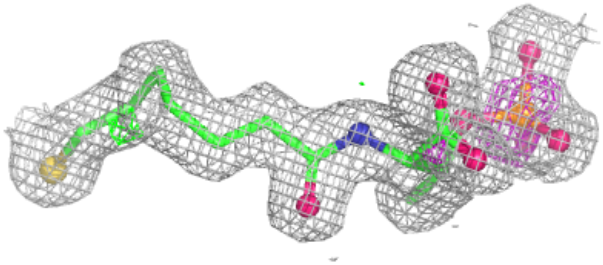


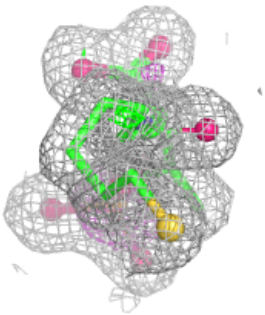


Electron density around TP7 D 1 (A):

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

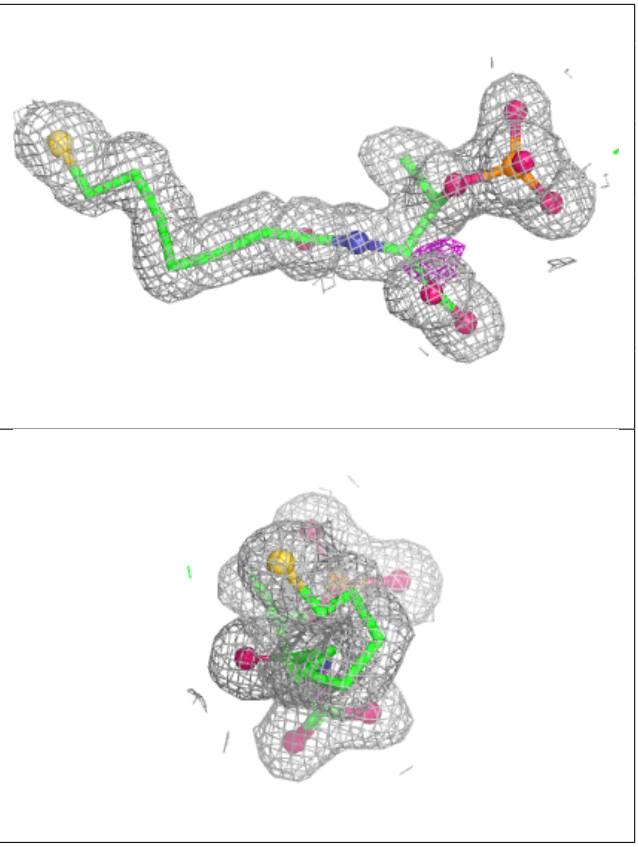






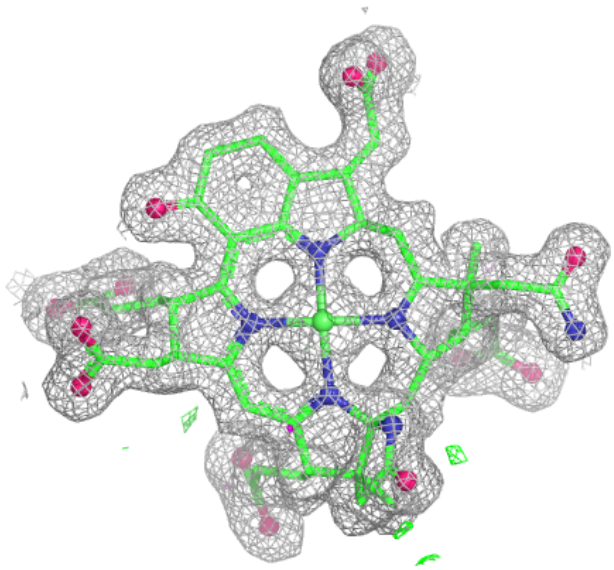
Electron density around TP7 A 552 (A):

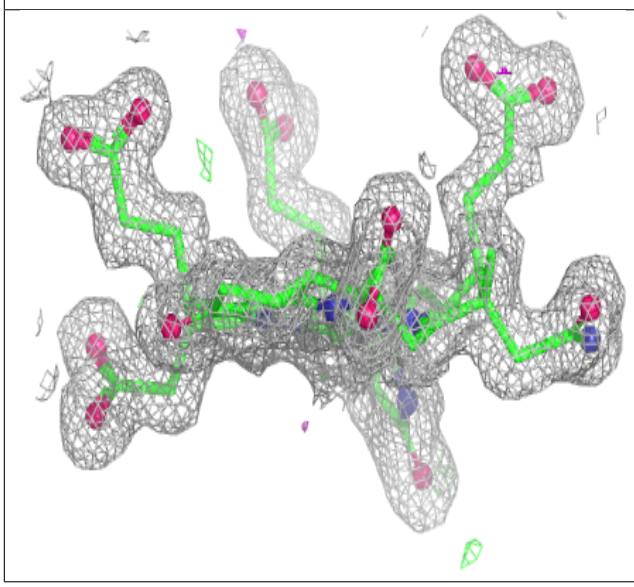
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

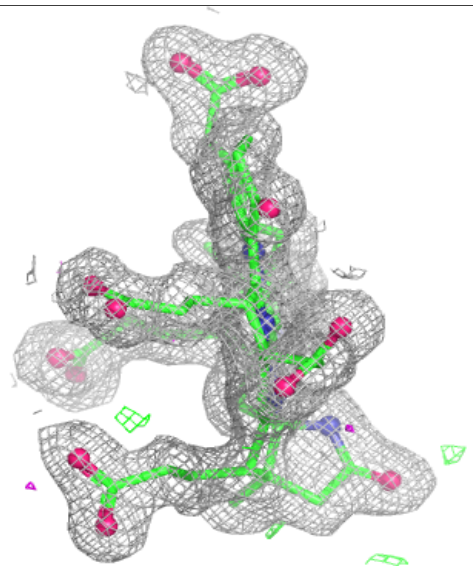


Electron density around F43 A 1:

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







Electron density around F43 D 551:

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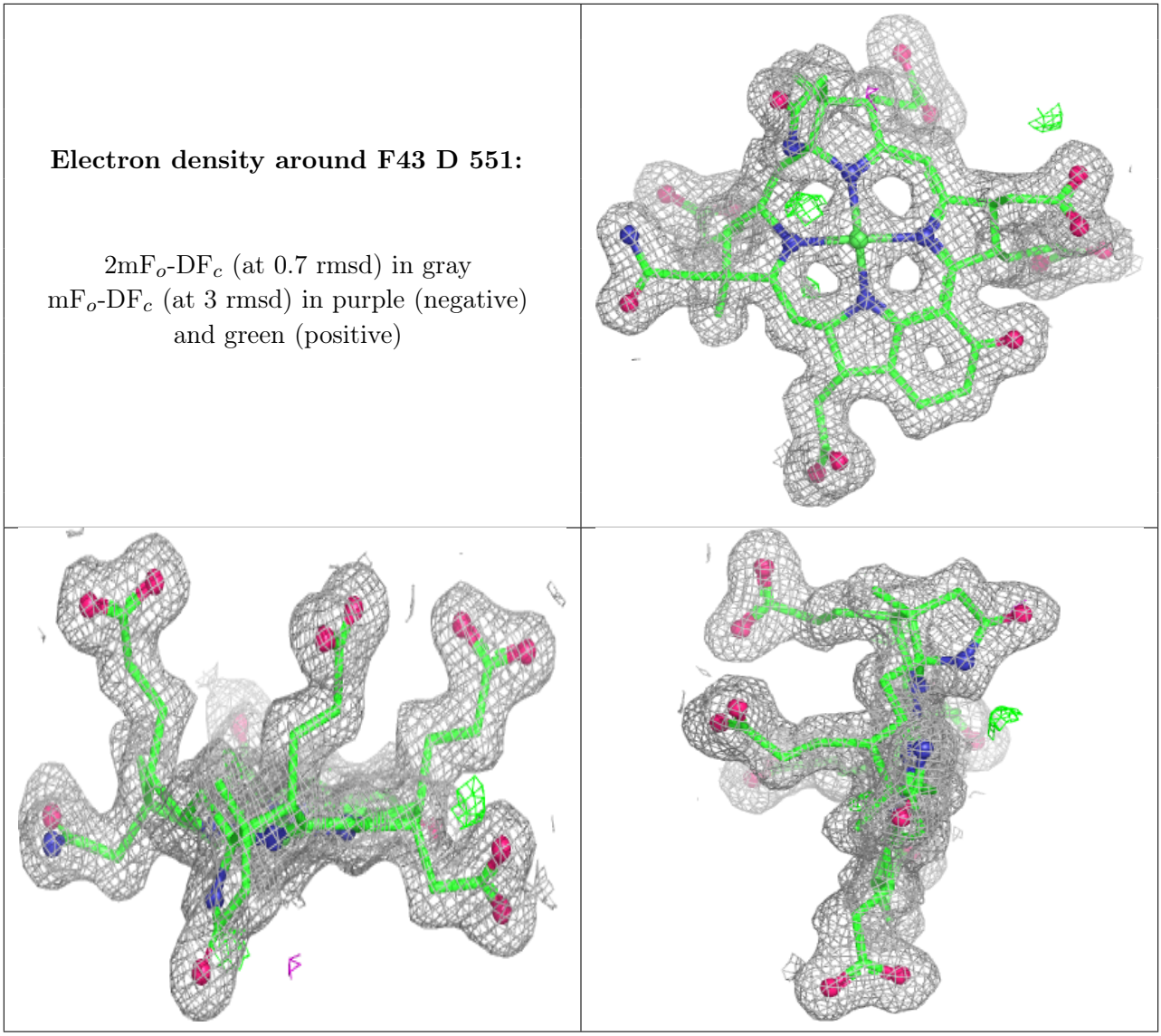
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.