



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 02:29 PM JST

PDB ID : 8Z75
Title : The structure of non-activated thiocyanate dehydrogenase from *Pelomicrobium methylotrophicum* (pmTcDH)
Authors : Varfolomeeva, L.A.; Solovieva, A.Y.; Shipkov, N.S.; Dergousova, N.I.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.
Deposited on : 2024-04-19
Resolution : 1.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

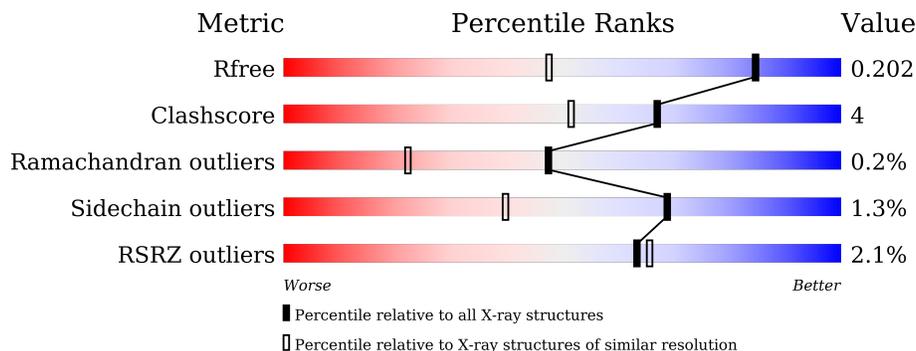
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	489	 2% 87% 7% • 5%
1	B	489	 2% 87% 7% • 5%
1	C	489	 2% 84% 10% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12307 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 Twin-arginine translocation signal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	Total 3650	C 2350	N 613	O 671	S 16	0	11	0
1	B	463	Total 3644	C 2341	N 619	O 670	S 14	6	12	0
1	C	463	Total 3636	C 2339	N 614	O 669	S 14	8	10	0

There are 63 discrepancies between the modelled and reference sequences:

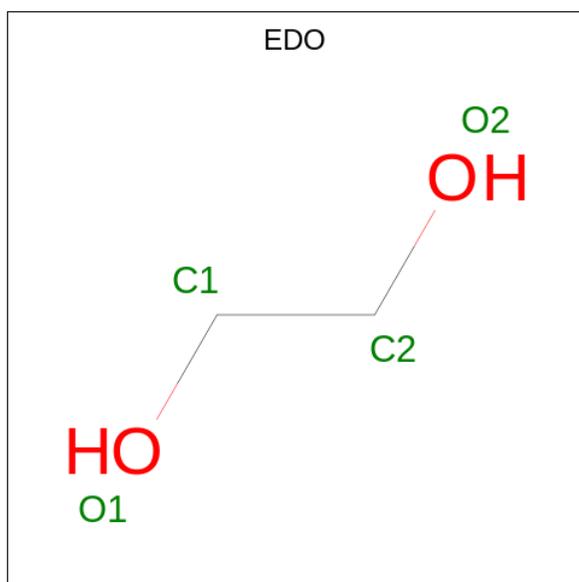
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP A0A5C7ETD9
A	26	GLY	-	expression tag	UNP A0A5C7ETD9
A	27	SER	-	expression tag	UNP A0A5C7ETD9
A	28	ASP	-	expression tag	UNP A0A5C7ETD9
A	29	LYS	-	expression tag	UNP A0A5C7ETD9
A	30	ILE	-	expression tag	UNP A0A5C7ETD9
A	31	HIS	-	expression tag	UNP A0A5C7ETD9
A	32	HIS	-	expression tag	UNP A0A5C7ETD9
A	33	HIS	-	expression tag	UNP A0A5C7ETD9
A	34	HIS	-	expression tag	UNP A0A5C7ETD9
A	35	HIS	-	expression tag	UNP A0A5C7ETD9
A	36	HIS	-	expression tag	UNP A0A5C7ETD9
A	37	GLU	-	expression tag	UNP A0A5C7ETD9
A	38	ASN	-	expression tag	UNP A0A5C7ETD9
A	39	LEU	-	expression tag	UNP A0A5C7ETD9
A	40	TYR	-	expression tag	UNP A0A5C7ETD9
A	41	PHE	-	expression tag	UNP A0A5C7ETD9
A	42	GLN	-	expression tag	UNP A0A5C7ETD9
A	43	GLY	-	expression tag	UNP A0A5C7ETD9
A	44	HIS	-	expression tag	UNP A0A5C7ETD9
A	45	MET	-	expression tag	UNP A0A5C7ETD9
B	25	MET	-	initiating methionine	UNP A0A5C7ETD9
B	26	GLY	-	expression tag	UNP A0A5C7ETD9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	SER	-	expression tag	UNP A0A5C7ETD9
B	28	ASP	-	expression tag	UNP A0A5C7ETD9
B	29	LYS	-	expression tag	UNP A0A5C7ETD9
B	30	ILE	-	expression tag	UNP A0A5C7ETD9
B	31	HIS	-	expression tag	UNP A0A5C7ETD9
B	32	HIS	-	expression tag	UNP A0A5C7ETD9
B	33	HIS	-	expression tag	UNP A0A5C7ETD9
B	34	HIS	-	expression tag	UNP A0A5C7ETD9
B	35	HIS	-	expression tag	UNP A0A5C7ETD9
B	36	HIS	-	expression tag	UNP A0A5C7ETD9
B	37	GLU	-	expression tag	UNP A0A5C7ETD9
B	38	ASN	-	expression tag	UNP A0A5C7ETD9
B	39	LEU	-	expression tag	UNP A0A5C7ETD9
B	40	TYR	-	expression tag	UNP A0A5C7ETD9
B	41	PHE	-	expression tag	UNP A0A5C7ETD9
B	42	GLN	-	expression tag	UNP A0A5C7ETD9
B	43	GLY	-	expression tag	UNP A0A5C7ETD9
B	44	HIS	-	expression tag	UNP A0A5C7ETD9
B	45	MET	-	expression tag	UNP A0A5C7ETD9
C	25	MET	-	initiating methionine	UNP A0A5C7ETD9
C	26	GLY	-	expression tag	UNP A0A5C7ETD9
C	27	SER	-	expression tag	UNP A0A5C7ETD9
C	28	ASP	-	expression tag	UNP A0A5C7ETD9
C	29	LYS	-	expression tag	UNP A0A5C7ETD9
C	30	ILE	-	expression tag	UNP A0A5C7ETD9
C	31	HIS	-	expression tag	UNP A0A5C7ETD9
C	32	HIS	-	expression tag	UNP A0A5C7ETD9
C	33	HIS	-	expression tag	UNP A0A5C7ETD9
C	34	HIS	-	expression tag	UNP A0A5C7ETD9
C	35	HIS	-	expression tag	UNP A0A5C7ETD9
C	36	HIS	-	expression tag	UNP A0A5C7ETD9
C	37	GLU	-	expression tag	UNP A0A5C7ETD9
C	38	ASN	-	expression tag	UNP A0A5C7ETD9
C	39	LEU	-	expression tag	UNP A0A5C7ETD9
C	40	TYR	-	expression tag	UNP A0A5C7ETD9
C	41	PHE	-	expression tag	UNP A0A5C7ETD9
C	42	GLN	-	expression tag	UNP A0A5C7ETD9
C	43	GLY	-	expression tag	UNP A0A5C7ETD9
C	44	HIS	-	expression tag	UNP A0A5C7ETD9
C	45	MET	-	expression tag	UNP A0A5C7ETD9

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

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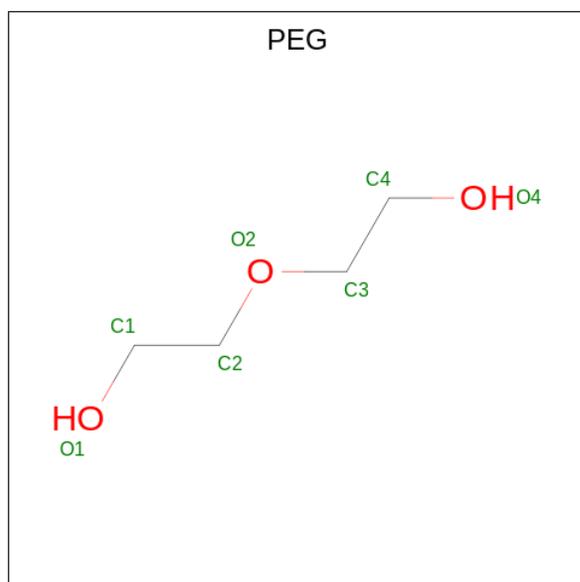
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0
4	B	1	Total Cu 1 1	0	0
4	C	1	Total Cu 1 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 4 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	473	Total O 473 473	0	0

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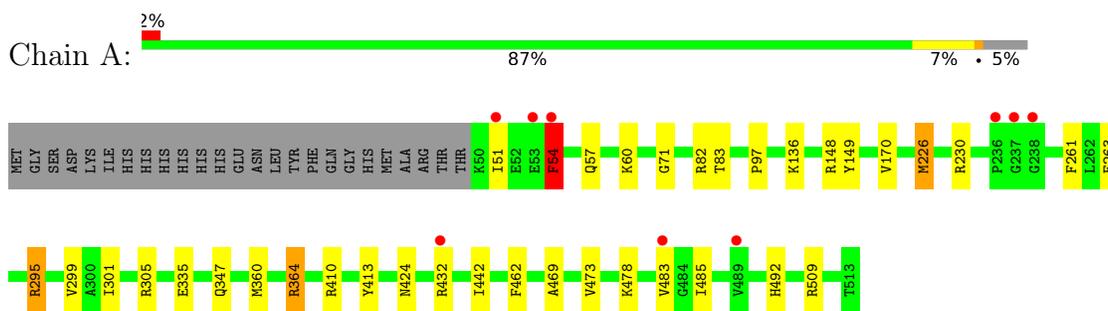
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	454	Total 454	O 454	0	0
6	C	398	Total 398	O 398	0	0

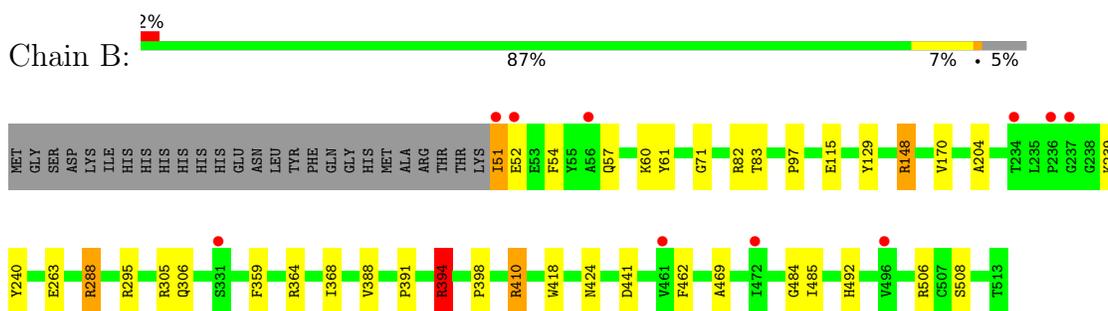
3 Residue-property plots [i](#)

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.

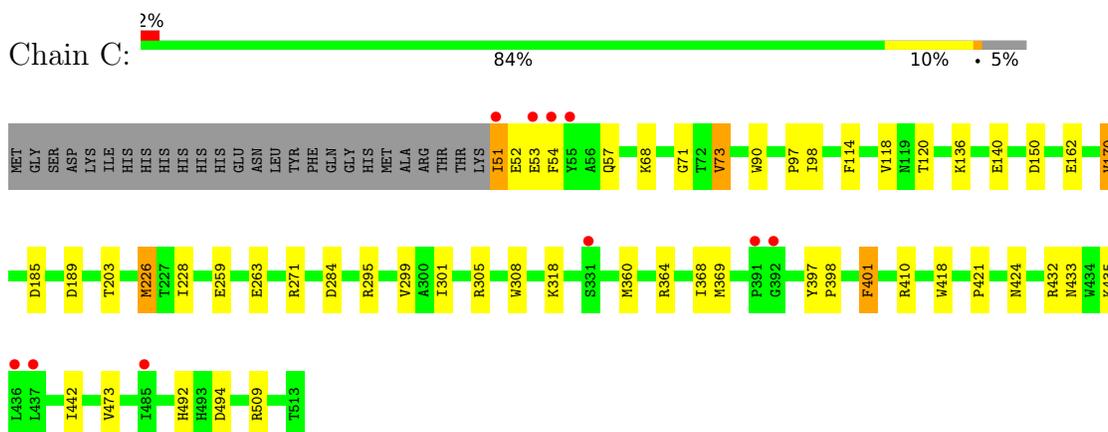
- Molecule 1: Twin-arginine translocation signal domain-containing protein



- Molecule 1: Twin-arginine translocation signal domain-containing protein



- Molecule 1: Twin-arginine translocation signal domain-containing protein



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.99Å 101.95Å 276.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 1.45 49.00 – 1.44	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.04-1.45) 99.4 (49.00-1.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.196 0.173 , 0.202	Depositor DCC
R_{free} test set	14079 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12307	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CU, PEG, 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	0.78	0/3807	1.20	14/5182 (0.3%)
1	B	0.82	3/3804 (0.1%)	1.24	23/5177 (0.4%)
1	C	0.83	4/3786 (0.1%)	1.25	17/5155 (0.3%)
All	All	0.81	7/11397 (0.1%)	1.23	54/15514 (0.3%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	GLU	CB-CG	17.14	1.84	1.52
1	B	52	GLU	CB-CG	11.04	1.73	1.52
1	C	52	GLU	CB-CG	-9.81	1.33	1.52
1	C	259	GLU	CD-OE2	6.12	1.32	1.25
1	B	51	ILE	CB-CG2	-5.93	1.34	1.52
1	C	140	GLU	CD-OE1	-5.38	1.19	1.25
1	B	508	SER	CB-OG	5.37	1.49	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	GLU	CA-CB-CG	-10.59	90.10	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PHE	CB-CA-C	8.92	128.24	110.40
1	C	509	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	295	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	401	PHE	CB-CG-CD2	7.75	126.22	120.80
1	A	295	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	148[A]	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	B	148[B]	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	B	288	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	364	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	51	ILE	CG1-CB-CG2	-7.12	95.74	111.40
1	C	295	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	C	52	GLU	CA-CB-CG	6.75	128.26	113.40
1	B	410	ARG	CG-CD-NE	6.65	125.76	111.80
1	C	305	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	509	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	148[A]	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	B	148[B]	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	C	150	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	B	204	ALA	N-CA-CB	6.17	118.74	110.10
1	B	148[A]	ARG	CD-NE-CZ	6.17	132.23	123.60
1	B	148[B]	ARG	CD-NE-CZ	6.17	132.23	123.60
1	A	413	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	B	394	ARG	CB-CG-CD	6.06	127.35	111.60
1	B	305	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	397	TYR	CB-CG-CD2	5.90	124.54	121.00
1	A	299	VAL	CA-CB-CG1	5.86	119.68	110.90
1	C	401	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	A	148	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	B	129	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	C	295	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	284	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	A	149	TYR	CB-CG-CD2	5.54	124.33	121.00
1	C	494	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	364	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	230	ARG	CG-CD-NE	-5.37	100.52	111.80
1	B	441	ASP	CB-CA-C	-5.35	99.70	110.40
1	A	509	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	61	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	305	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	261	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	B	359	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	C	68	LYS	CB-CA-C	5.24	120.88	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	TYR	CB-CG-CD1	5.22	124.13	121.00
1	C	90	TRP	CD1-NE1-CE2	-5.16	104.36	109.00
1	B	305	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	271	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	359	PHE	CB-CG-CD1	5.08	124.35	120.80
1	C	189	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	148	ARG	CD-NE-CZ	5.06	130.68	123.60
1	B	506	ARG	CG-CD-NE	-5.02	101.25	111.80
1	C	114	PHE	CB-CG-CD2	5.02	124.31	120.80
1	B	115[A]	GLU	CB-CA-C	-5.00	100.39	110.40
1	B	115[B]	GLU	CB-CA-C	-5.00	100.39	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain
1	A	462	PHE	Peptide
1	B	462	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3650	0	3595	36	0
1	B	3644	0	3594	27	0
1	C	3636	0	3587	30	0
2	A	8	0	11	0	0
2	B	16	0	24	0	0
2	C	16	0	23	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	6	0	7	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	473	0	0	8	0
6	B	454	0	0	10	0
6	C	398	0	0	3	0
All	All	12307	0	10841	85	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 (85) 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:B:82[A]:ARG:NH2	6:B:703:HOH:O	1.61	1.32
1:C:410:ARG:HH11	1:C:432:ARG:NH2	1.37	1.21
1:B:82[A]:ARG:CZ	6:B:703:HOH:O	1.84	1.18
1:A:60:LYS:NZ	6:A:703:HOH:O	1.74	1.15
1:B:82[A]:ARG:NE	6:B:703:HOH:O	1.80	1.10
1:A:82[B]:ARG:NH2	6:A:702:HOH:O	1.56	1.08
1:A:54:PHE:CE1	1:B:51:ILE:HB	1.90	1.07
1:A:82[B]:ARG:NE	6:A:702:HOH:O	1.94	1.01
1:C:410:ARG:NH1	1:C:432:ARG:NH2	2.13	0.95
1:C:410:ARG:NH1	1:C:432:ARG:CZ	2.31	0.94
1:B:82[A]:ARG:NH2	6:B:704:HOH:O	2.01	0.93
1:A:263:GLU:OE1	1:A:364:ARG:NH2	2.01	0.92
1:A:410:ARG:NH1	1:A:432:ARG:HH21	1.76	0.84
1:C:54:PHE:O	1:C:57:GLN:HG2	1.76	0.84
1:B:263:GLU:OE1	1:B:364[A]:ARG:NH2	2.12	0.83
1:A:60:LYS:HE3	6:A:843:HOH:O	1.78	0.82
1:C:410:ARG:HH11	1:C:432:ARG:CZ	1.93	0.80
1:A:54:PHE:O	1:A:57:GLN:HG2	1.82	0.80
1:A:226[B]:MET:SD	1:A:301:ILE:HD11	2.24	0.78
1:C:410:ARG:HH11	1:C:432:ARG:HH21	1.28	0.78
1:A:82[B]:ARG:CZ	6:A:702:HOH:O	1.98	0.77
5:C:603:PEG:H32	6:C:1016:HOH:O	1.85	0.76
1:C:226[B]:MET:SD	1:C:301:ILE:HD11	2.26	0.76
1:B:60:LYS:HE3	6:B:1090:HOH:O	1.85	0.74
1:C:263:GLU:OE1	1:C:364[A]:ARG:NH2	2.18	0.74
1:A:410:ARG:HH12	1:A:432:ARG:NH2	1.87	0.72
1:A:335[A]:GLU:OE2	6:A:704:HOH:O	2.09	0.71
1:B:239:LYS:HE3	6:B:909:HOH:O	1.90	0.70
1:A:54:PHE:HE1	1:A:483:VAL:HG23	1.57	0.69
1:B:239:LYS:CE	6:B:909:HOH:O	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148[B]:ARG:HD2	6:B:706:HOH:O	1.95	0.65
1:A:410:ARG:NH1	1:A:432:ARG:NH2	2.46	0.62
1:A:51:ILE:HG13	1:A:54:PHE:CD2	2.34	0.62
1:C:410:ARG:HH12	1:C:432:ARG:CZ	2.12	0.62
1:A:54:PHE:CE1	1:A:483:VAL:HG23	2.36	0.61
1:C:433[B]:ASN:OD1	1:C:435:LYS:HD3	2.01	0.61
1:A:60:LYS:CE	6:A:843:HOH:O	2.41	0.60
1:C:364[B]:ARG:NH1	6:C:703:HOH:O	2.34	0.60
1:B:60:LYS:CE	6:B:1090:HOH:O	2.47	0.58
1:B:391:PRO:HA	1:B:394:ARG:HD3	1.89	0.54
1:A:485[A]:ILE:CD1	1:B:82[A]:ARG:NH2	2.71	0.54
1:B:71:GLY:HA2	1:B:97:PRO:O	2.08	0.53
1:A:51:ILE:HD11	1:A:54:PHE:CE2	2.44	0.53
1:C:51:ILE:O	1:C:51:ILE:HG12	2.09	0.52
1:A:51:ILE:HG22	1:B:484:GLY:HA3	1.91	0.52
1:B:54:PHE:O	1:B:57:GLN:HG2	2.10	0.52
1:C:410:ARG:HG2	1:C:432:ARG:HD3	1.93	0.51
1:A:71:GLY:HA2	1:A:97:PRO:O	2.11	0.50
1:B:288:ARG:HD2	1:B:306:GLN:HG3	1.94	0.50
1:C:360:MET:SD	1:C:368:ILE:HG12	2.53	0.49
1:A:485[A]:ILE:CD1	1:B:82[A]:ARG:CZ	2.92	0.48
5:C:603:PEG:H21	5:C:603:PEG:H42	1.62	0.48
1:A:485[A]:ILE:HD11	1:B:82[A]:ARG:NH2	2.29	0.48
1:A:54:PHE:HA	1:A:57:GLN:OE1	2.13	0.47
1:C:162[B]:GLU:OE1	6:C:702:HOH:O	2.20	0.47
1:C:398:PRO:HD3	1:C:418:TRP:CH2	2.49	0.47
1:B:398:PRO:HD3	1:B:418:TRP:CZ2	2.49	0.47
1:C:410:ARG:NH1	1:C:432:ARG:NE	2.61	0.47
1:A:51:ILE:HG13	1:A:54:PHE:HD2	1.75	0.47
1:A:478:LYS:CE	6:A:855:HOH:O	2.62	0.46
1:C:442:ILE:HD12	1:C:473:VAL:HG21	1.97	0.46
1:C:71:GLY:HA2	1:C:97:PRO:O	2.16	0.46
1:C:433[B]:ASN:CG	1:C:435:LYS:HD3	2.37	0.45
1:A:82[B]:ARG:CZ	1:B:485:ILE:HD12	2.46	0.45
1:A:51:ILE:CG1	1:A:54:PHE:CD2	2.99	0.45
1:B:239:LYS:HE2	6:B:909:HOH:O	2.15	0.45
1:C:170:VAL:HG23	1:C:185:ASP:HA	1.98	0.44
1:A:51:ILE:CG1	1:A:54:PHE:HD2	2.31	0.43
1:B:368:ILE:HB	1:B:388:VAL:HB	2.01	0.43
1:A:54:PHE:CZ	1:B:51:ILE:HB	2.45	0.42
1:C:73[A]:VAL:CG1	1:C:118:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:CD1	1:B:51:ILE:HB	2.47	0.42
1:C:398:PRO:HD3	1:C:418:TRP:CZ2	2.55	0.41
1:A:442:ILE:HD12	1:A:473:VAL:HG21	2.01	0.41
1:A:83:THR:O	1:B:469:ALA:HA	2.20	0.41
1:A:136:LYS:HD3	1:A:136:LYS:HA	1.77	0.41
1:A:347:GLN:O	1:A:360[B]:MET:HG2	2.21	0.40
1:A:469:ALA:HA	1:B:83:THR:O	2.21	0.40
1:C:98:ILE:O	1:C:120:THR:HA	2.22	0.40
1:C:203:THR:HG21	1:C:308:TRP:CE3	2.56	0.40
1:C:318:LYS:HA	1:C:369:MET:HE3	2.03	0.40
1:C:226[B]:MET:HE1	1:C:299[B]:VAL:HG21	2.02	0.40
1:C:136:LYS:HA	1:C:136:LYS:HD3	1.88	0.40
1:C:410:ARG:HD3	1:C:432:ARG:NH2	2.36	0.40
1:C:228:ILE:HD11	1:C:301:ILE:HD13	2.03	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	473/489 (97%)	450 (95%)	22 (5%)	1 (0%)	47 22
1	B	473/489 (97%)	451 (95%)	21 (4%)	1 (0%)	47 22
1	C	471/489 (96%)	450 (96%)	20 (4%)	1 (0%)	47 22
All	All	1417/1467 (97%)	1351 (95%)	63 (4%)	3 (0%)	47 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	VAL
1	B	170	VAL
1	C	170	VAL

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	395/406 (97%)	390 (99%)	5 (1%)	69	40
1	B	395/406 (97%)	391 (99%)	4 (1%)	76	52
1	C	393/406 (97%)	384 (98%)	9 (2%)	50	17
All	All	1183/1218 (97%)	1165 (98%)	18 (2%)	69	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	PHE
1	A	226[A]	MET
1	A	226[B]	MET
1	A	424	ASN
1	A	492	HIS
1	B	394	ARG
1	B	410	ARG
1	B	424	ASN
1	B	492	HIS
1	C	51	ILE
1	C	73[A]	VAL
1	C	73[B]	VAL
1	C	226[A]	MET
1	C	226[B]	MET
1	C	401	PHE
1	C	421	PRO
1	C	424	ASN
1	C	492	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	GLN
1	B	306	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\# Z > 2$
2	EDO	C	602	-	3,3,3	0.11	0	2,2,2	0.70	0
2	EDO	B	604	-	3,3,3	0.19	0	2,2,2	0.31	0
2	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.83	0
2	EDO	A	601	-	3,3,3	0.56	0	2,2,2	0.24	0
5	PEG	C	603	-	5,5,6	0.32	0	4,4,5	0.72	0
2	EDO	A	602	-	3,3,3	0.84	0	2,2,2	0.41	0
2	EDO	C	601	-	3,3,3	0.97	0	2,2,2	0.65	0
2	EDO	C	604	-	3,3,3	0.62	0	2,2,2	0.36	0
2	EDO	C	605	-	3,3,3	0.41	0	2,2,2	0.18	0
2	EDO	B	601	-	3,3,3	0.80	0	2,2,2	0.30	0
2	EDO	B	603	-	3,3,3	0.27	0	2,2,2	0.51	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
2	EDO	C	602	-	-	1/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
5	PEG	C	603	-	-	3/3/3/4	-
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	C	601	-	-	1/1/1/1	-
2	EDO	C	604	-	-	0/1/1/1	-
2	EDO	C	605	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	603	PEG	C4-C3-O2-C2
5	C	603	PEG	O2-C3-C4-O4
2	A	602	EDO	O1-C1-C2-O2
2	C	602	EDO	O1-C1-C2-O2
5	C	603	PEG	C1-C2-O2-C3
2	C	601	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	603	PEG	2	0

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	464/489 (94%)	0.18	9 (1%) 66 68	12, 17, 27, 41	13 (2%)
1	B	463/489 (94%)	0.22	10 (2%) 62 65	12, 17, 27, 44	17 (3%)
1	C	463/489 (94%)	0.27	10 (2%) 62 65	13, 19, 31, 60	16 (3%)
All	All	1390/1467 (94%)	0.23	29 (2%) 63 65	12, 18, 29, 60	46 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	PHE	6.4
1	C	55	TYR	5.2
1	C	485	ILE	5.2
1	C	51	ILE	4.7
1	A	54	PHE	4.2
1	C	53	GLU	4.1
1	B	51	ILE	3.8
1	B	236	PRO	3.6
1	A	237	GLY	3.5
1	C	331	SER	3.5
1	B	56	ALA	3.4
1	A	236	PRO	3.0
1	C	437	LEU	2.8
1	B	331	SER	2.6
1	B	237	GLY	2.6
1	A	53	GLU	2.6
1	A	432	ARG	2.5
1	A	483	VAL	2.5
1	B	234	THR	2.4
1	A	238	GLY	2.4
1	C	392	GLY	2.4
1	C	391	PRO	2.4
1	B	472	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	489	VAL	2.2
1	C	436	LEU	2.1
1	B	461	VAL	2.1
1	A	51	ILE	2.1
1	B	496[A]	VAL	2.0
1	B	52	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

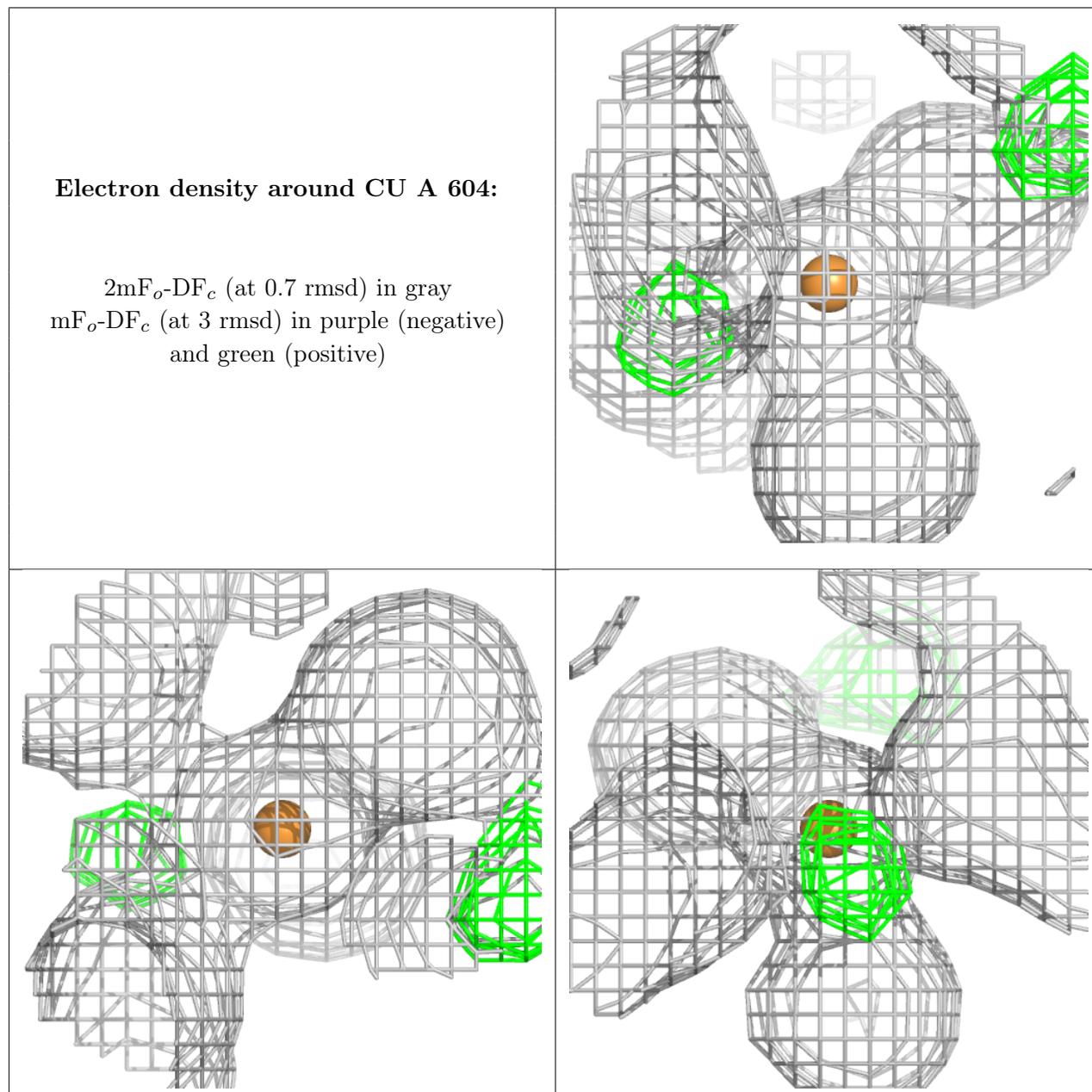
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

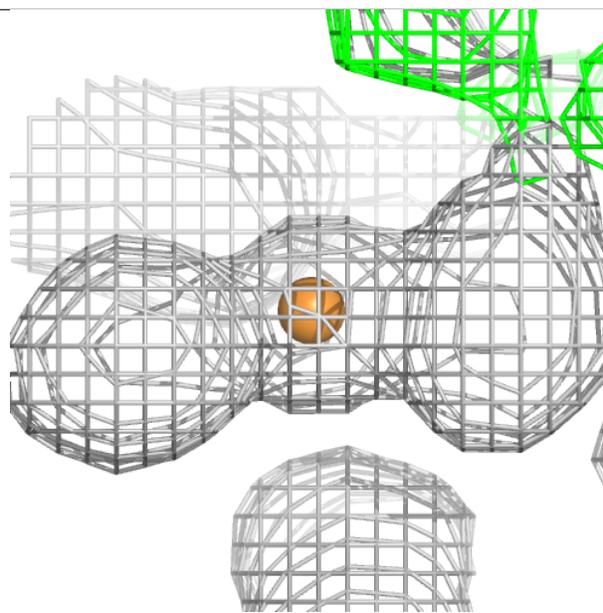
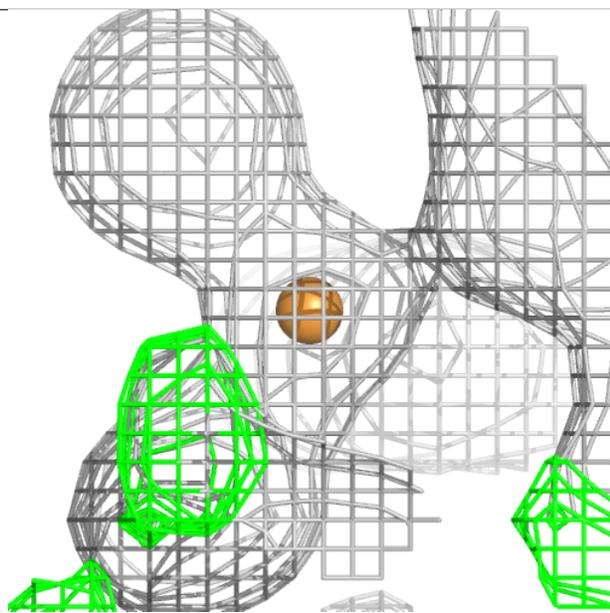
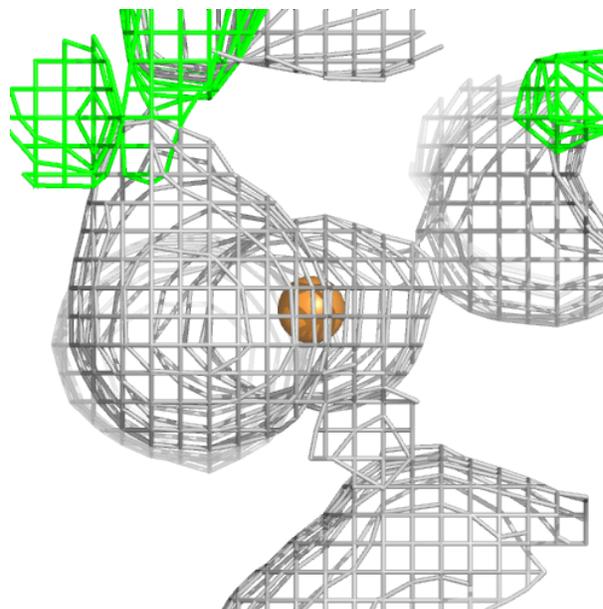
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	C	605	4/4	0.76	0.30	25,31,32,34	4
5	PEG	C	603	6/7	0.84	0.30	15,21,21,24	6
2	EDO	B	601	4/4	0.86	0.14	22,22,24,25	0
2	EDO	A	602	4/4	0.94	0.09	19,23,26,33	0
2	EDO	C	604	4/4	0.94	0.07	21,22,22,22	0
2	EDO	A	601	4/4	0.95	0.12	17,19,19,19	0
2	EDO	B	602	4/4	0.95	0.07	20,20,20,24	0
3	CL	B	605	1/1	0.95	0.13	23,23,23,23	1
2	EDO	B	603	4/4	0.95	0.33	17,19,19,25	4
2	EDO	C	601	4/4	0.96	0.10	17,19,19,25	4
2	EDO	C	602	4/4	0.96	0.28	18,19,20,20	4
4	CU	A	604	1/1	0.96	0.08	16,16,16,16	1
2	EDO	B	604	4/4	0.96	0.17	19,20,22,23	4
4	CU	B	606	1/1	0.98	0.12	15,15,15,15	1
4	CU	C	607	1/1	0.98	0.13	21,21,21,21	1
3	CL	A	603	1/1	0.98	0.11	21,21,21,21	1
3	CL	C	606	1/1	0.99	0.07	25,25,25,25	0

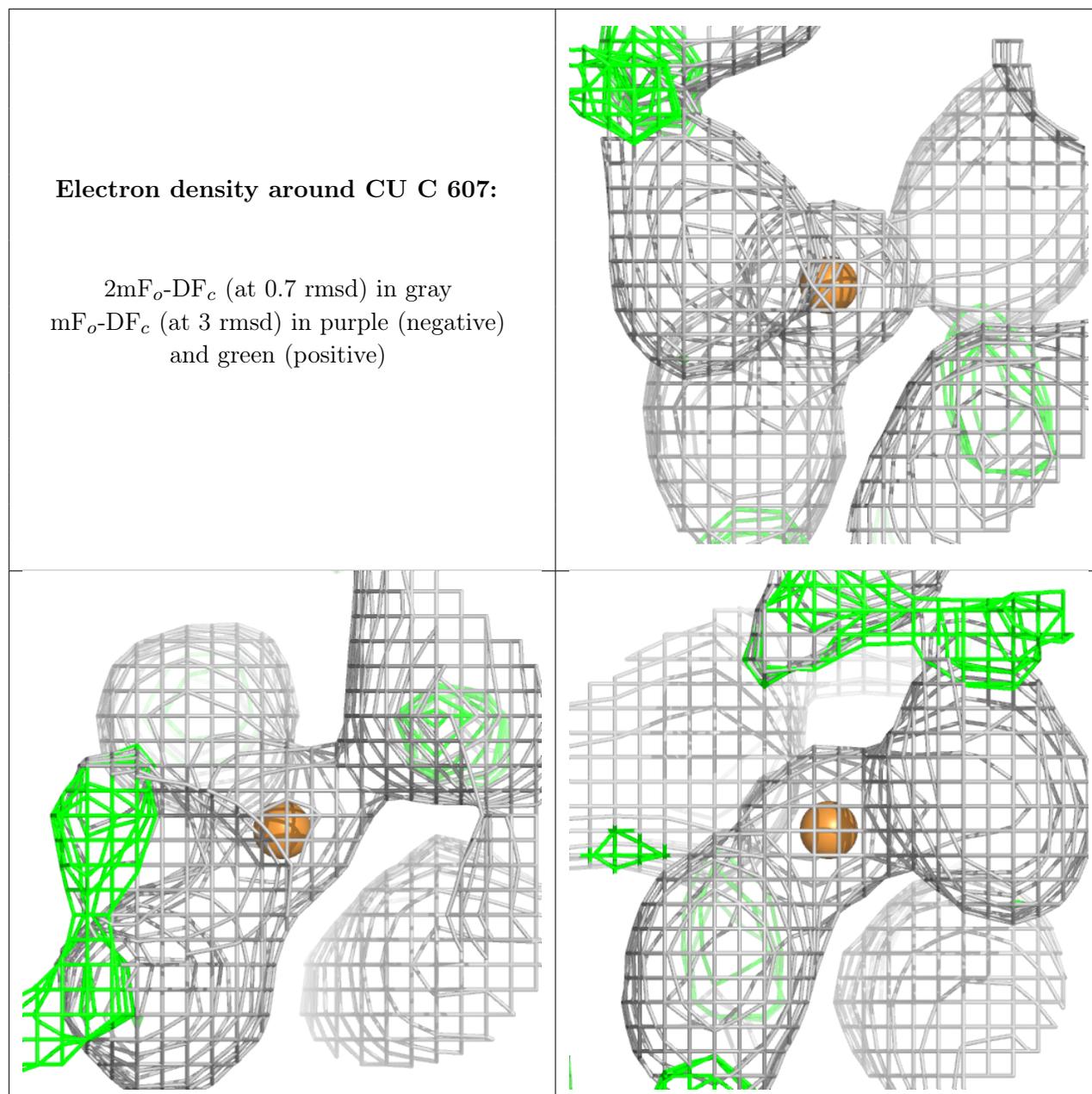
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around CU B 606:

$2mF_o-DF_c$ (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.