



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:57 PM UTC

PDB ID : 6I3Q / pdb_00006i3q
Title : The structure of thiocyanate dehydrogenase from Thioalkalivibrio paradoxus complex with acetate ions.
Authors : Polyakov, K.M.; Popov, A.N.; Tikhkonova, T.V.; Popov, V.O.; Trofimov, A.A.
Deposited on : 2018-11-07
Resolution : 1.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

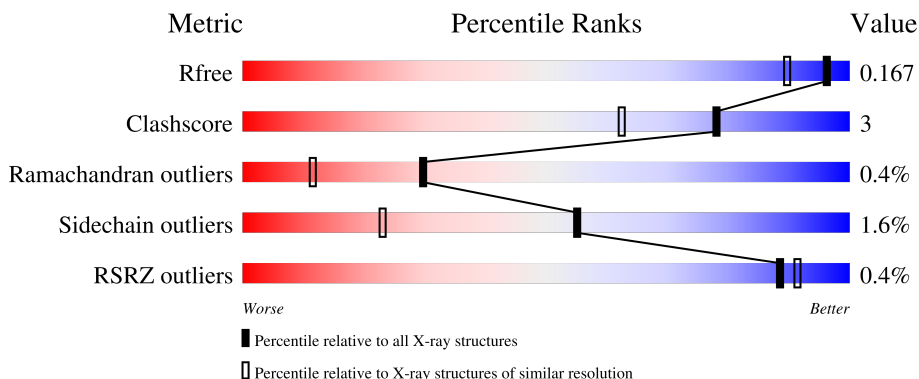
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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

Mol	Chain	Length	Quality of chain
1	A	548	79% 5% 15%
1	B	548	% 78% 7% 15%
1	C	548	79% 6% 15%
1	D	548	78% 7% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16357 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.

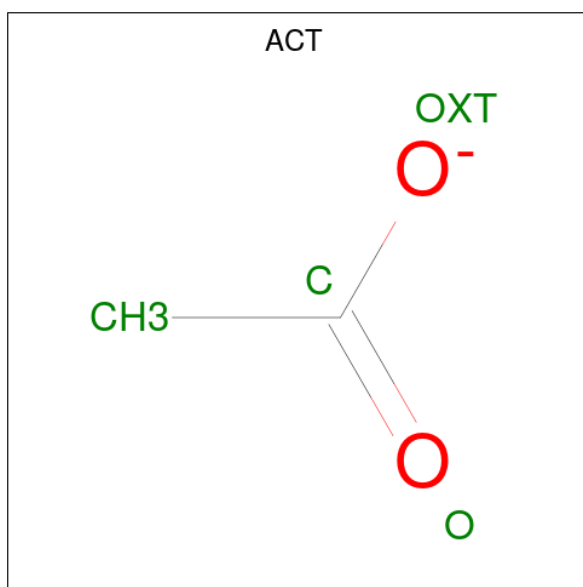
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	11	0
			3663	2337	607	699	20			
1	B	467	Total	C	N	O	S	0	8	0
			3653	2329	607	696	21			
1	C	466	Total	C	N	O	S	0	7	0
			3645	2327	604	695	19			
1	D	467	Total	C	N	O	S	0	13	0
			3671	2343	610	699	19			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		
2	D	2	Total	Cu	0	0
			2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



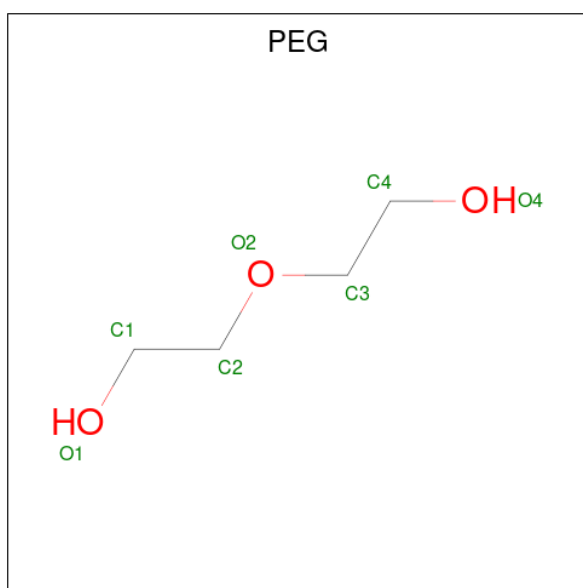
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			5	3	2		

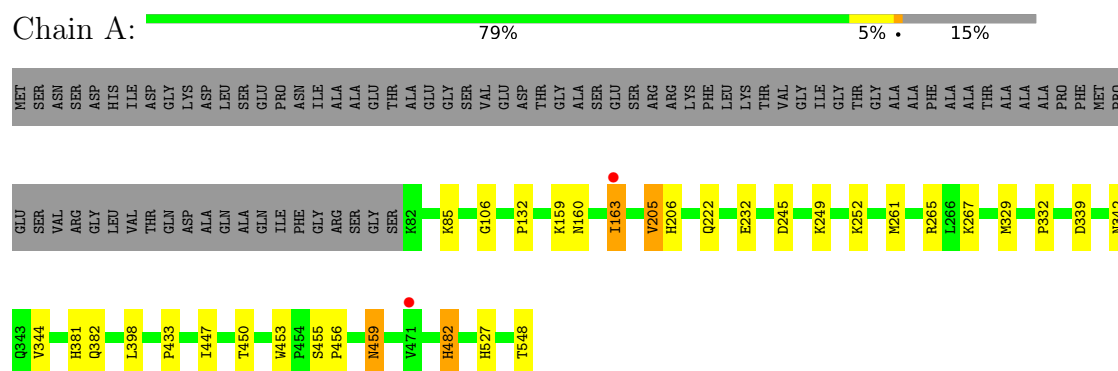
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	412	Total 412	O 412	0	0
6	B	401	Total 401	O 401	0	0
6	C	436	Total 436	O 436	0	0
6	D	415	Total 415	O 415	0	0

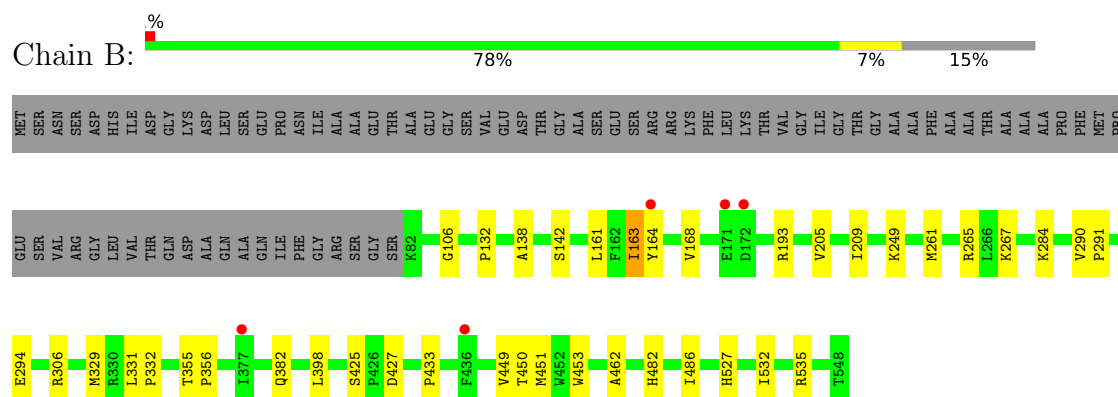
3 Residue-property plots [i](#)

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.

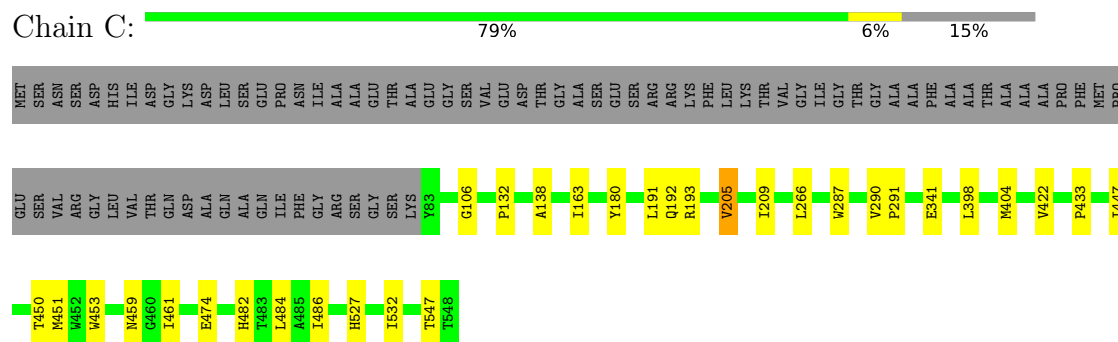
• Molecule 1: Uncharacterized protein



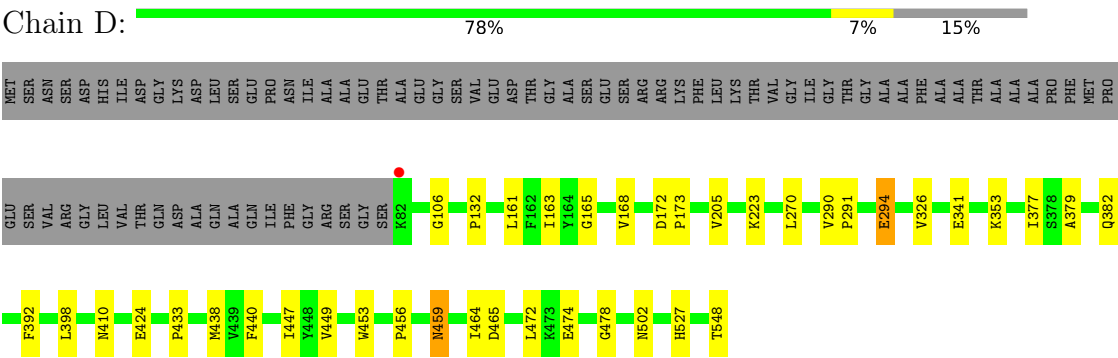
• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein



● Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.96Å 162.70Å 90.94Å 90.00° 119.93° 90.00°	Depositor
Resolution (Å)	45.48 – 1.45 45.48 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.48-1.45) 99.8 (45.48-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.142 , 0.165 0.151 , 0.167	Depositor DCC
R_{free} test set	20017 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,k,-h-l 0.015 for -h-l,k,h 0.046 for -h-l,-k,l 0.013 for h,-k,-h-l 0.148 for l,-k,h	Xtriage
Reported twinning fraction	0.439 for H, K, L 0.561 for L, -K, H	Depositor
Outliers	0 of 402549 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16357	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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: CU, GOL, PEG, ACT

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	0.85	1/3827 (0.0%)	1.00	2/5219 (0.0%)
1	B	0.84	0/3799	1.00	2/5183 (0.0%)
1	C	0.86	0/3786	0.97	0/5167
1	D	0.83	0/3842	0.99	2/5244 (0.0%)
All	All	0.85	1/15254 (0.0%)	0.99	6/20813 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	HIS	CA-C	-7.99	1.49	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	VAL	CA-C-N	-5.34	114.74	120.03
1	A	344	VAL	C-N-CA	-5.34	114.74	120.03
1	B	331	LEU	CA-C-N	-5.17	114.63	120.89
1	B	331	LEU	C-N-CA	-5.17	114.63	120.89
1	D	270	LEU	CA-C-N	-5.05	114.52	119.92

There are no chirality outliers.

There are no planarity outliers.

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	3663	0	3521	19	0
1	B	3653	0	3518	18	0
1	C	3645	0	3510	18	0
1	D	3671	0	3514	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	8	0	1	0	0
3	B	8	0	2	0	0
3	C	8	0	2	0	0
3	D	12	0	9	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	D	5	0	5	1	0
6	A	412	0	0	3	0
6	B	401	0	0	0	0
6	C	436	0	0	1	0
6	D	415	0	0	2	0
All	All	16357	0	14098	80	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 3.

The worst 5 of 80 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:A:382:GLN:HG3	6:A:758:HOH:O	1.43	1.15
1:D:290:VAL:HG22	1:D:291:PRO:HD2	1.47	0.96
1:D:290:VAL:HG22	1:D:291:PRO:CD	1.96	0.95
1:C:451:MET:HG3	1:C:474:GLU:OE1	1.79	0.82
1:D:438:MET:SD	1:D:447[A]:ILE:HD11	2.22	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/548 (87%)	448 (94%)	26 (6%)	2 (0%)	30	11
1	B	473/548 (86%)	448 (95%)	23 (5%)	2 (0%)	30	11
1	C	471/548 (86%)	446 (95%)	23 (5%)	2 (0%)	30	11
1	D	478/548 (87%)	450 (94%)	26 (5%)	2 (0%)	30	11
All	All	1898/2192 (87%)	1792 (94%)	98 (5%)	8 (0%)	30	11

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	LEU
1	C	205	VAL
1	C	398	LEU
1	D	205	VAL
1	A	205	VAL

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	402/451 (89%)	396 (98%)	6 (2%)	57	25
1	B	398/451 (88%)	392 (98%)	6 (2%)	57	25
1	C	397/451 (88%)	391 (98%)	6 (2%)	57	25
1	D	402/451 (89%)	394 (98%)	8 (2%)	48	16
All	All	1599/1804 (89%)	1573 (98%)	26 (2%)	55	23

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	447	ILE
1	C	547	THR
1	D	474	GLU

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Mol	Chain	Res	Type
1	C	527	HIS
1	D	163	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	ASN
1	D	342	ASN
1	D	468	ASN
1	D	382	GLN
1	D	390	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\# Z > 2$
3	ACT	D	604	2	3,3,3	0.86	0	3,3,3	0.48	0
3	ACT	D	603	2	3,3,3	0.79	0	3,3,3	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	606	-	5,5,5	0.23	0	5,5,5	0.63	0
3	ACT	B	604	2,3	3,3,3	0.79	0	3,3,3	1.01	0
4	GOL	C	605	-	5,5,5	0.47	0	5,5,5	0.23	0
3	ACT	A	603	2,3	3,3,3	0.73	0	3,3,3	0.72	0
3	ACT	C	604	2,3	3,3,3	1.12	0	3,3,3	1.05	0
5	PEG	D	607	-	4,4,6	0.35	0	3,3,5	0.44	0
3	ACT	A	604	2,3	3,3,3	0.70	0	3,3,3	1.84	1 (33%)
3	ACT	D	605	-	3,3,3	0.86	0	3,3,3	0.74	0
3	ACT	B	603	2,3	3,3,3	1.03	0	3,3,3	0.73	0
3	ACT	C	603	2,3	3,3,3	0.73	0	3,3,3	0.65	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
4	GOL	C	605	-	-	0/4/4/4	-
5	PEG	D	607	-	-	2/2/2/4	-
4	GOL	D	606	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	ACT	OXT-C-CH3	2.54	125.71	115.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	607	PEG	O2-C3-C4-O4
5	D	607	PEG	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	605	GOL	1	0
5	D	607	PEG	1	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	467/548 (85%)	-0.06	2 (0%) 88 91	10, 16, 25, 40	10 (2%)
1	B	467/548 (85%)	-0.05	5 (1%) 78 82	10, 17, 25, 37	8 (1%)
1	C	466/548 (85%)	-0.16	0 100 100	10, 15, 23, 30	7 (1%)
1	D	467/548 (85%)	-0.21	1 (0%) 91 93	9, 15, 23, 34	13 (2%)
All	All	1867/2192 (85%)	-0.12	8 (0%) 88 91	9, 16, 24, 40	38 (2%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	ASP	4.2
1	B	164	TYR	2.5
1	D	82	LYS	2.3
1	B	377	ILE	2.3
1	B	436	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	D	605	4/4	0.77	0.32	19,20,20,21	4
3	ACT	D	604	4/4	0.88	0.22	16,18,18,19	4
3	ACT	C	604	4/4	0.88	0.21	12,13,14,15	4
5	PEG	D	607	5/7	0.88	0.17	17,18,19,19	5
4	GOL	D	606	6/6	0.90	0.11	11,12,14,14	6
3	ACT	A	603	4/4	0.90	0.13	15,16,16,16	4
3	ACT	C	603	4/4	0.91	0.15	12,12,13,14	4
3	ACT	A	604	4/4	0.92	0.13	14,14,15,17	4
3	ACT	B	604	4/4	0.93	0.16	16,16,16,16	4
3	ACT	D	603	4/4	0.93	0.13	14,14,14,15	4
3	ACT	B	603	4/4	0.94	0.10	11,12,12,13	4
4	GOL	C	605	6/6	0.97	0.06	15,18,18,19	0
2	CU	C	601	1/1	1.00	0.02	16,16,16,16	0
2	CU	C	602	1/1	1.00	0.01	14,14,14,14	1
2	CU	D	601	1/1	1.00	0.02	16,16,16,16	0
2	CU	D	602	1/1	1.00	0.01	13,13,13,13	1
2	CU	A	601	1/1	1.00	0.02	17,17,17,17	0
2	CU	A	602	1/1	1.00	0.01	15,15,15,15	1
2	CU	B	601	1/1	1.00	0.01	17,17,17,17	0
2	CU	B	602	1/1	1.00	0.01	14,14,14,14	1

6.5 Other polymers [i](#)

There are no such residues in this entry.