



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:06 AM UTC

PDB ID : 8SF6 / pdb_00008sf6
Title : Promiscuous amino acid gamma synthase from *Caldicellulosiruptor hydrothermalis* in closed conformation
Authors : Buller, A.R.; Zmich, A.P.; Bingman, C.A.
Deposited on : 2023-04-10
Resolution : 1.70 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

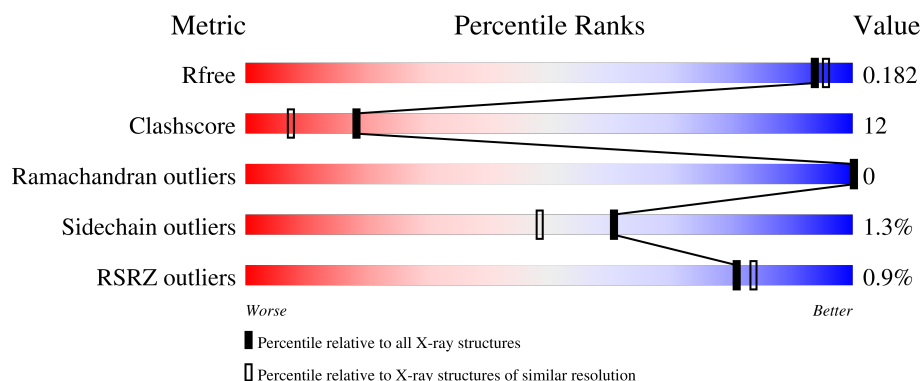
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	433	
1	B	433	
1	C	433	
1	D	433	
1	E	433	

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Mol	Chain	Length	Quality of chain
1	F	433	
1	G	433	
1	H	433	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28751 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 O-acetylhomoserine/O-acetylserine sulfhydrylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	P	S	0	6	0
			3342	2157	550	629	1	5			
1	B	424	Total	C	N	O	P	S	0	4	0
			3332	2151	552	623	1	5			
1	C	423	Total	C	N	O	P	S	0	4	0
			3328	2150	551	621	1	5			
1	D	424	Total	C	N	O	P	S	0	2	0
			3322	2143	548	624	1	6			
1	E	425	Total	C	N	O	P	S	0	4	0
			3328	2150	553	619	1	5			
1	F	423	Total	C	N	O	P	S	0	1	0
			3283	2122	541	614	1	5			
1	G	423	Total	C	N	O	P	S	0	3	0
			3317	2140	547	624	1	5			
1	H	425	Total	C	N	O	P	S	0	2	0
			3305	2135	544	620	1	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	LEU	-	expression tag	UNP E4QC33
A	427	GLU	-	expression tag	UNP E4QC33
A	428	HIS	-	expression tag	UNP E4QC33
A	429	HIS	-	expression tag	UNP E4QC33
A	430	HIS	-	expression tag	UNP E4QC33
A	431	HIS	-	expression tag	UNP E4QC33
A	432	HIS	-	expression tag	UNP E4QC33
A	433	HIS	-	expression tag	UNP E4QC33
B	426	LEU	-	expression tag	UNP E4QC33
B	427	GLU	-	expression tag	UNP E4QC33
B	428	HIS	-	expression tag	UNP E4QC33
B	429	HIS	-	expression tag	UNP E4QC33
B	430	HIS	-	expression tag	UNP E4QC33

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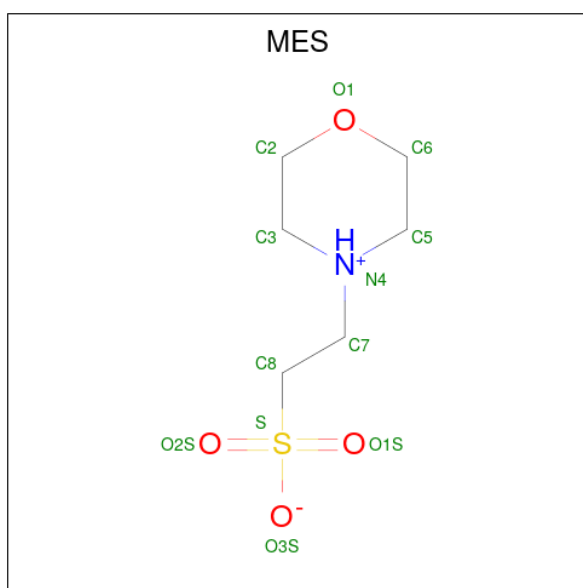
Chain	Residue	Modelled	Actual	Comment	Reference
B	431	HIS	-	expression tag	UNP E4QC33
B	432	HIS	-	expression tag	UNP E4QC33
B	433	HIS	-	expression tag	UNP E4QC33
C	426	LEU	-	expression tag	UNP E4QC33
C	427	GLU	-	expression tag	UNP E4QC33
C	428	HIS	-	expression tag	UNP E4QC33
C	429	HIS	-	expression tag	UNP E4QC33
C	430	HIS	-	expression tag	UNP E4QC33
C	431	HIS	-	expression tag	UNP E4QC33
C	432	HIS	-	expression tag	UNP E4QC33
C	433	HIS	-	expression tag	UNP E4QC33
D	426	LEU	-	expression tag	UNP E4QC33
D	427	GLU	-	expression tag	UNP E4QC33
D	428	HIS	-	expression tag	UNP E4QC33
D	429	HIS	-	expression tag	UNP E4QC33
D	430	HIS	-	expression tag	UNP E4QC33
D	431	HIS	-	expression tag	UNP E4QC33
D	432	HIS	-	expression tag	UNP E4QC33
D	433	HIS	-	expression tag	UNP E4QC33
E	426	LEU	-	expression tag	UNP E4QC33
E	427	GLU	-	expression tag	UNP E4QC33
E	428	HIS	-	expression tag	UNP E4QC33
E	429	HIS	-	expression tag	UNP E4QC33
E	430	HIS	-	expression tag	UNP E4QC33
E	431	HIS	-	expression tag	UNP E4QC33
E	432	HIS	-	expression tag	UNP E4QC33
E	433	HIS	-	expression tag	UNP E4QC33
F	426	LEU	-	expression tag	UNP E4QC33
F	427	GLU	-	expression tag	UNP E4QC33
F	428	HIS	-	expression tag	UNP E4QC33
F	429	HIS	-	expression tag	UNP E4QC33
F	430	HIS	-	expression tag	UNP E4QC33
F	431	HIS	-	expression tag	UNP E4QC33
F	432	HIS	-	expression tag	UNP E4QC33
F	433	HIS	-	expression tag	UNP E4QC33
G	426	LEU	-	expression tag	UNP E4QC33
G	427	GLU	-	expression tag	UNP E4QC33
G	428	HIS	-	expression tag	UNP E4QC33
G	429	HIS	-	expression tag	UNP E4QC33
G	430	HIS	-	expression tag	UNP E4QC33
G	431	HIS	-	expression tag	UNP E4QC33
G	432	HIS	-	expression tag	UNP E4QC33

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Chain	Residue	Modelled	Actual	Comment	Reference
G	433	HIS	-	expression tag	UNP E4QC33
H	426	LEU	-	expression tag	UNP E4QC33
H	427	GLU	-	expression tag	UNP E4QC33
H	428	HIS	-	expression tag	UNP E4QC33
H	429	HIS	-	expression tag	UNP E4QC33
H	430	HIS	-	expression tag	UNP E4QC33
H	431	HIS	-	expression tag	UNP E4QC33
H	432	HIS	-	expression tag	UNP E4QC33
H	433	HIS	-	expression tag	UNP E4QC33

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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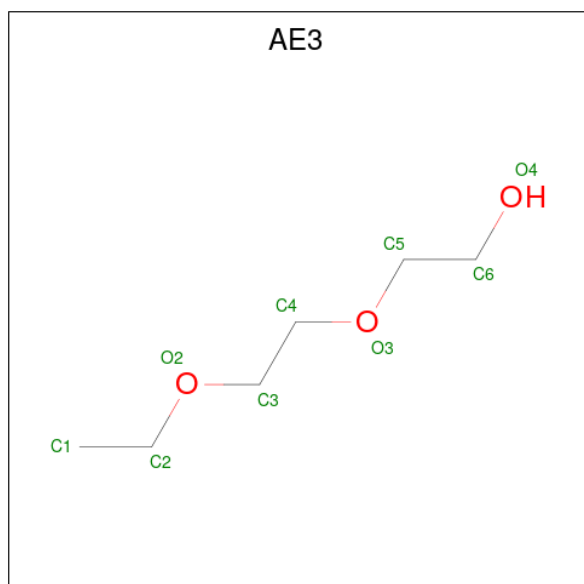
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is 2-(2-ETHOXYETHOXY)ETHANOL (CCD ID: AE3) (formula: C₆H₁₄O₃).



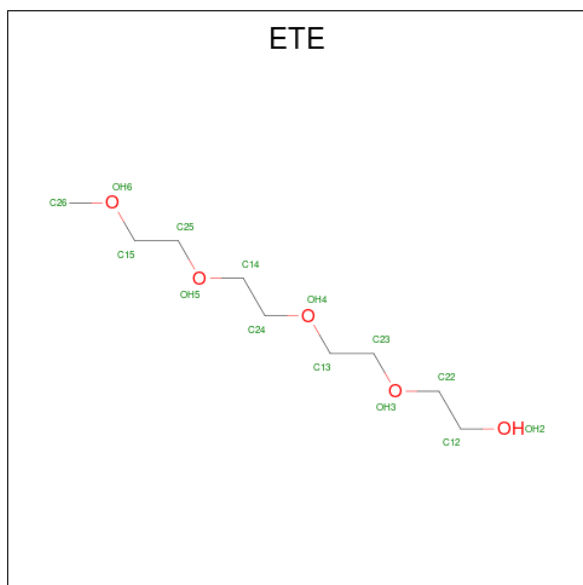
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			9	6	3		

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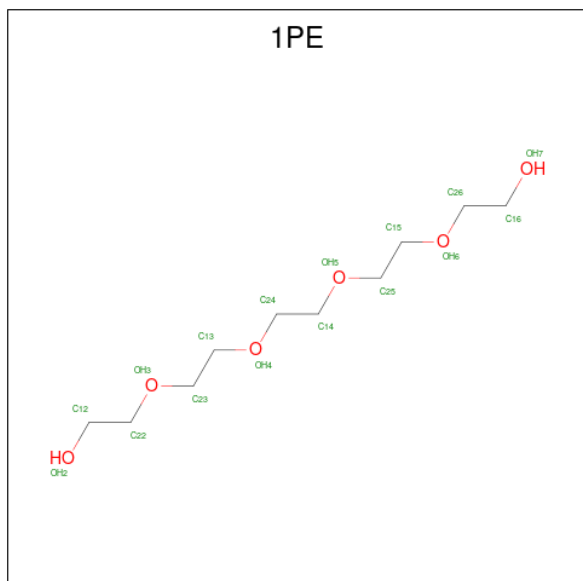
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			9	6	3		

- Molecule 5 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			14	9	5		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			16	10	6		
6	H	1	Total	C	O	0	0
			16	10	6		

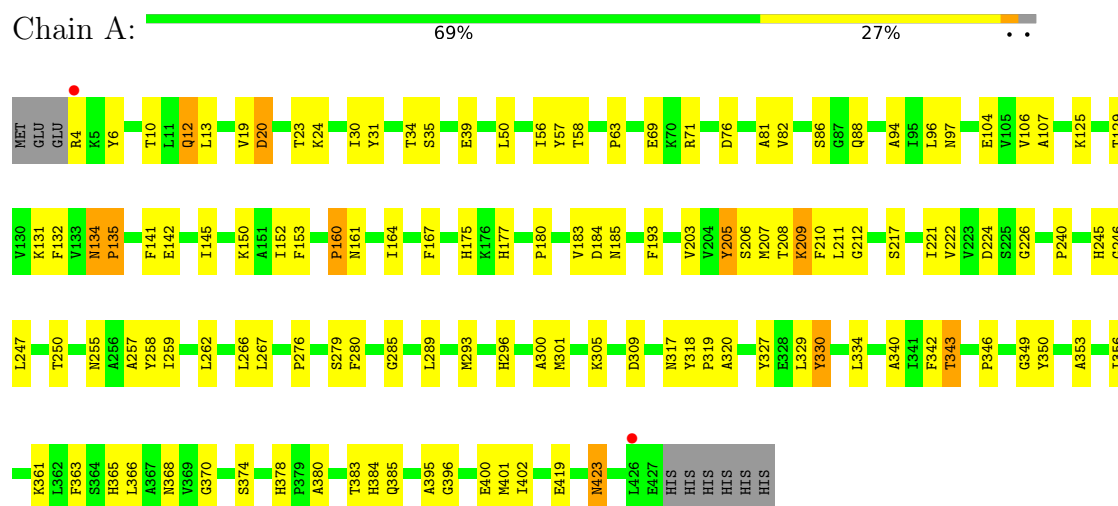
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	264	Total	O	0	0
			264	264		
7	B	284	Total	O	0	0
			284	284		
7	C	259	Total	O	0	0
			259	259		
7	D	237	Total	O	0	0
			237	237		
7	E	251	Total	O	0	0
			251	251		
7	F	156	Total	O	0	0
			156	156		
7	G	284	Total	O	0	0
			284	284		
7	H	286	Total	O	0	0
			286	286		

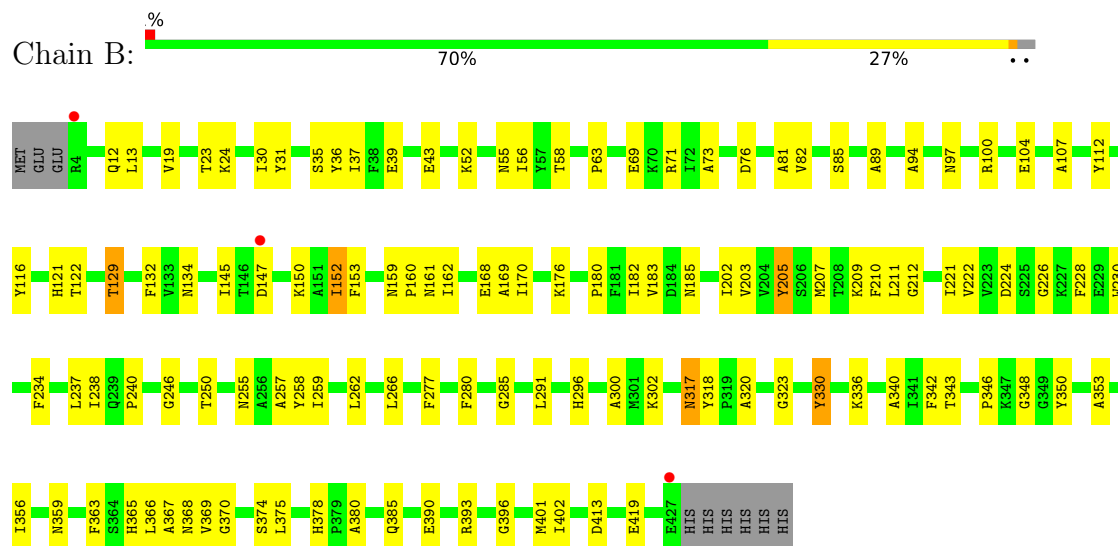
3 Residue-property plots

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

- Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



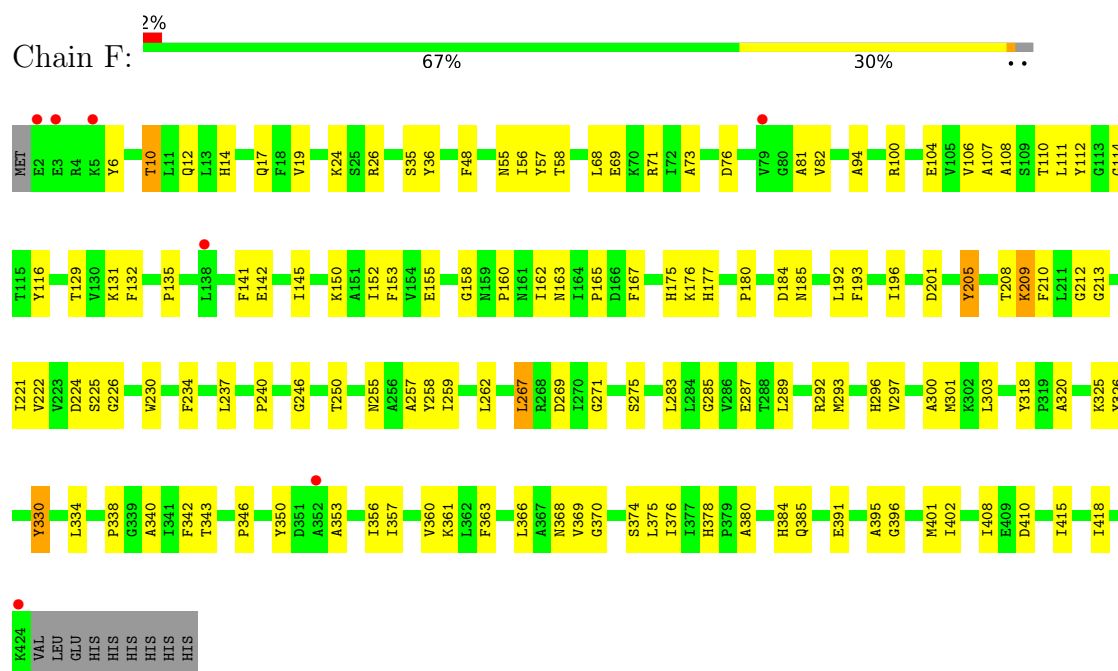
- Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



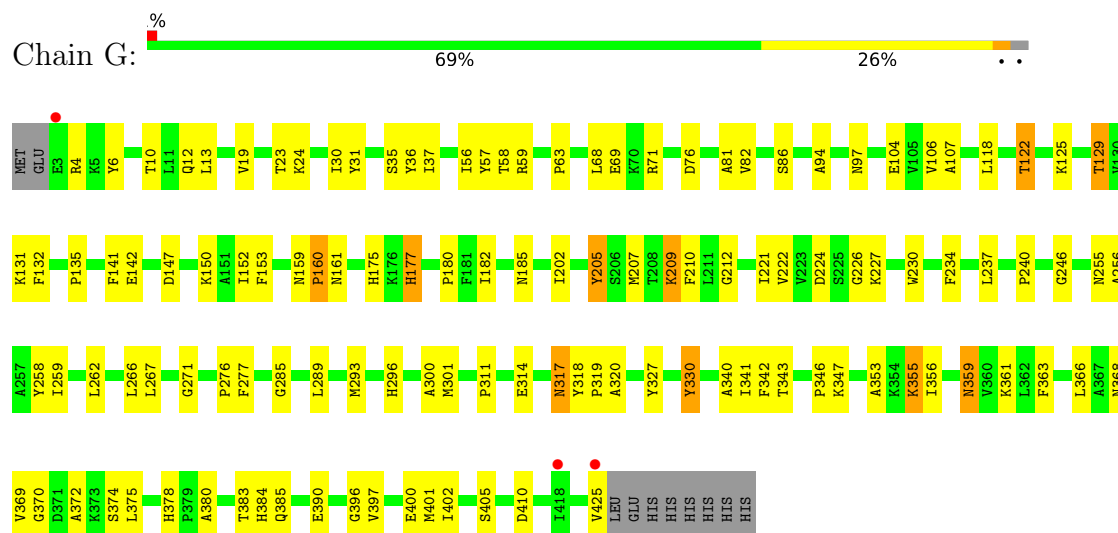
- Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase





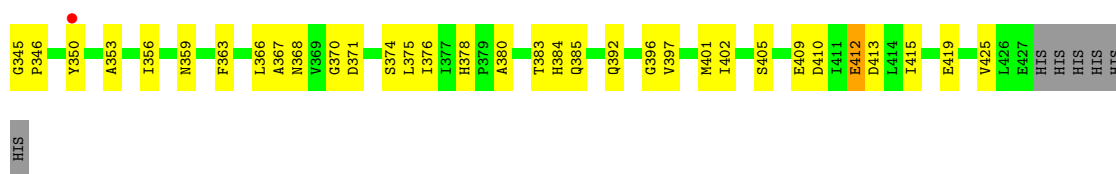


- Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase



- Molecule 1: O-acetylhomoserine/O-acetylserine sulfhydrylase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	279.09Å 133.12Å 115.79Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	39.92 – 1.70 39.92 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.92-1.70) 97.2 (39.92-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.154 , 0.179 0.159 , 0.182	Depositor DCC
R_{free} test set	22101 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	28751	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: LLP, MES, NA, AE3, 1PE, ETE

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	1.23	4/3400 (0.1%)	1.45	16/4619 (0.3%)
1	B	1.30	3/3387 (0.1%)	1.45	20/4601 (0.4%)
1	C	1.27	5/3386 (0.1%)	1.46	13/4598 (0.3%)
1	D	1.26	5/3374 (0.1%)	1.42	16/4582 (0.3%)
1	E	1.25	5/3389 (0.1%)	1.43	15/4603 (0.3%)
1	F	1.07	2/3335 (0.1%)	1.44	13/4536 (0.3%)
1	G	1.30	3/3372 (0.1%)	1.44	15/4582 (0.3%)
1	H	1.36	11/3360 (0.3%)	1.47	19/4568 (0.4%)
All	All	1.26	38/27003 (0.1%)	1.45	127/36689 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	269	ASP	C-O	-8.09	1.14	1.24
1	C	206	SER	CA-CB	-6.47	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	13	LEU	C-O	-6.21	1.15	1.23
1	H	376	ILE	C-N	-6.19	1.30	1.33
1	E	206	SER	CA-CB	-6.09	1.45	1.52

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ASN	CB-CA-C	8.50	126.87	109.95
1	C	58	THR	CA-CB-OG1	-7.95	97.68	109.60
1	E	58	THR	CA-CB-OG1	-7.66	98.12	109.60
1	G	129	THR	CA-CB-OG1	-7.23	98.75	109.60
1	A	423	ASN	N-CA-C	-7.15	104.53	113.18

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Peptide
1	B	205	TYR	Peptide
1	C	205	TYR	Peptide
1	D	205	TYR	Peptide
1	E	205	TYR	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	3342	0	3314	86	0
1	B	3332	0	3311	81	0
1	C	3328	0	3321	74	0
1	D	3322	0	3297	96	0
1	E	3328	0	3315	82	0
1	F	3283	0	3240	90	0
1	G	3317	0	3287	91	0
1	H	3305	0	3267	92	0
2	A	12	0	13	3	0
2	B	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	13	1	0
2	D	12	0	13	1	0
2	E	12	0	13	2	0
2	F	12	0	13	2	0
2	G	12	0	13	3	0
2	H	12	0	13	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	D	9	0	14	0	0
4	E	9	0	14	0	0
5	E	14	0	20	1	0
6	H	32	0	44	1	0
7	A	264	0	0	1	0
7	B	284	0	0	6	0
7	C	259	0	0	4	0
7	D	237	0	0	1	0
7	E	251	0	0	3	0
7	F	156	0	0	3	0
7	G	284	0	0	2	0
7	H	286	0	0	6	0
All	All	28751	0	26548	647	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 12.

The worst 5 of 647 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:H:410:ASP:OD1	1:H:412:GLU:OE1	1.99	0.81
1:E:161:ASN:O	1:E:317:ASN:ND2	2.21	0.74
1:F:353:ALA:HA	1:F:402:ILE:HD11	1.71	0.71
1:F:210:PHE:CE1	1:F:370:GLY:HA2	2.26	0.71
1:E:210:PHE:CE1	1:E:370:GLY:HA2	2.27	0.70

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	427/433 (99%)	417 (98%)	10 (2%)	0	100	100
1	B	425/433 (98%)	415 (98%)	10 (2%)	0	100	100
1	C	424/433 (98%)	414 (98%)	10 (2%)	0	100	100
1	D	423/433 (98%)	413 (98%)	10 (2%)	0	100	100
1	E	426/433 (98%)	414 (97%)	12 (3%)	0	100	100
1	F	421/433 (97%)	411 (98%)	10 (2%)	0	100	100
1	G	423/433 (98%)	415 (98%)	8 (2%)	0	100	100
1	H	424/433 (98%)	414 (98%)	10 (2%)	0	100	100
All	All	3393/3464 (98%)	3313 (98%)	80 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	349/358 (98%)	344 (99%)	5 (1%)	59	46
1	B	347/358 (97%)	344 (99%)	3 (1%)	70	62
1	C	348/358 (97%)	344 (99%)	4 (1%)	65	54
1	D	346/358 (97%)	340 (98%)	6 (2%)	53	38
1	E	346/358 (97%)	342 (99%)	4 (1%)	63	51
1	F	338/358 (94%)	335 (99%)	3 (1%)	70	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	346/358 (97%)	341 (99%)	5 (1%)	59	46
1	H	342/358 (96%)	337 (98%)	5 (2%)	57	43
All	All	2762/2864 (96%)	2727 (99%)	35 (1%)	61	48

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	410	ASP
1	G	425	VAL
1	H	160	PRO
1	D	1	MET
1	C	379	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	GLN
1	F	359	ASN
1	H	161	ASN
1	H	32	GLN
1	D	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	LLP	D	209	1	23,24,25	0.99	1 (4%)	25,32,34	1.00	1 (4%)
1	LLP	C	209	1	23,24,25	0.92	0	25,32,34	0.90	1 (4%)
1	LLP	F	209	1	23,24,25	0.82	0	25,32,34	1.10	1 (4%)
1	LLP	E	209	1	23,24,25	0.92	1 (4%)	25,32,34	0.87	1 (4%)
1	LLP	H	209	1	23,24,25	1.01	1 (4%)	25,32,34	0.93	1 (4%)
1	LLP	G	209	1	23,24,25	1.23	3 (13%)	25,32,34	0.91	2 (8%)
1	LLP	A	209	1	23,24,25	1.03	2 (8%)	25,32,34	0.94	1 (4%)
1	LLP	B	209	1	23,24,25	0.95	0	25,32,34	0.95	1 (4%)

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	LLP	D	209	1	-	2/16/17/19	0/1/1/1
1	LLP	C	209	1	-	2/16/17/19	0/1/1/1
1	LLP	F	209	1	-	3/16/17/19	0/1/1/1
1	LLP	E	209	1	-	4/16/17/19	0/1/1/1
1	LLP	H	209	1	-	4/16/17/19	0/1/1/1
1	LLP	G	209	1	-	2/16/17/19	0/1/1/1
1	LLP	A	209	1	-	3/16/17/19	0/1/1/1
1	LLP	B	209	1	-	3/16/17/19	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	209	LLP	C4-C5	-2.66	1.38	1.42
1	G	209	LLP	C3-C2	-2.48	1.38	1.41
1	E	209	LLP	C4-C5	-2.46	1.38	1.42
1	A	209	LLP	O3-C3	-2.21	1.31	1.36
1	G	209	LLP	P-OP3	-2.21	1.46	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	209	LLP	OP3-P-OP4	-3.15	98.45	106.67
1	B	209	LLP	OP2-P-OP4	-3.10	98.59	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LLP	OP2-P-OP4	-3.04	98.74	106.67
1	G	209	LLP	OP3-P-OP4	-2.90	99.10	106.67
1	C	209	LLP	OP4-P-OP1	-2.69	99.17	106.44

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	209	LLP	O-C-CA-CB
1	B	209	LLP	O-C-CA-CB
1	C	209	LLP	O-C-CA-CB
1	D	209	LLP	O-C-CA-CB
1	E	209	LLP	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	209	LLP	1	0
1	C	209	LLP	2	0
1	F	209	LLP	2	0
1	H	209	LLP	1	0
1	G	209	LLP	1	0
1	A	209	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 13 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	1PE	H	503	-	15,15,15	0.43	0	14,14,14	0.56	0
2	MES	H	501	-	12,12,12	0.85	0	15,16,16	0.80	0
2	MES	B	501	-	12,12,12	0.83	0	15,16,16	0.93	0
2	MES	F	501	-	12,12,12	0.64	0	15,16,16	0.70	0
2	MES	A	501	-	12,12,12	0.78	0	15,16,16	0.81	0
5	ETE	E	502	-	13,13,13	0.65	0	12,12,12	0.42	0
2	MES	D	501	-	12,12,12	0.70	0	15,16,16	0.71	0
4	AE3	E	503	-	8,8,8	0.58	0	7,7,7	0.34	0
2	MES	C	501	-	12,12,12	0.85	0	15,16,16	0.96	1 (6%)
2	MES	G	501	-	12,12,12	0.79	0	15,16,16	1.04	1 (6%)
4	AE3	D	502	-	8,8,8	0.53	0	7,7,7	0.39	0
6	1PE	H	502	-	15,15,15	0.49	0	14,14,14	0.48	0
2	MES	E	501	-	12,12,12	0.61	0	15,16,16	0.74	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	1PE	H	503	-	-	5/13/13/13	-
2	MES	H	501	-	-	6/6/14/14	0/1/1/1
2	MES	B	501	-	-	6/6/14/14	0/1/1/1
2	MES	F	501	-	-	6/6/14/14	0/1/1/1
2	MES	A	501	-	-	0/6/14/14	0/1/1/1
5	ETE	E	502	-	-	4/11/11/11	-
2	MES	D	501	-	-	0/6/14/14	0/1/1/1
4	AE3	E	503	-	-	3/6/6/6	-
2	MES	C	501	-	-	2/6/14/14	0/1/1/1
2	MES	G	501	-	-	0/6/14/14	0/1/1/1
4	AE3	D	502	-	-	3/6/6/6	-
6	1PE	H	502	-	-	6/13/13/13	-
2	MES	E	501	-	-	6/6/14/14	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	MES	O1S-S-C8	-2.24	103.35	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MES	O1S-S-C8	-2.10	103.55	106.73

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	MES	C8-C7-N4-C3
2	F	501	MES	C8-C7-N4-C5
2	F	501	MES	C7-C8-S-O1S
2	F	501	MES	C7-C8-S-O2S
2	H	501	MES	N4-C7-C8-S

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	503	1PE	1	0
2	H	501	MES	2	0
2	B	501	MES	1	0
2	F	501	MES	2	0
2	A	501	MES	3	0
5	E	502	ETE	1	0
2	D	501	MES	1	0
2	C	501	MES	1	0
2	G	501	MES	3	0
2	E	501	MES	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	423/433 (97%)	-0.08	2 (0%) 87 89	14, 30, 47, 68	6 (1%)
1	B	423/433 (97%)	-0.21	3 (0%) 84 86	13, 29, 42, 67	4 (0%)
1	C	422/433 (97%)	-0.15	3 (0%) 84 86	13, 30, 46, 72	4 (0%)
1	D	423/433 (97%)	-0.06	6 (1%) 73 77	12, 31, 49, 83	2 (0%)
1	E	424/433 (97%)	-0.13	5 (1%) 76 80	12, 31, 46, 75	4 (0%)
1	F	422/433 (97%)	0.23	7 (1%) 69 73	19, 38, 55, 84	1 (0%)
1	G	422/433 (97%)	-0.19	3 (0%) 84 86	13, 29, 44, 77	3 (0%)
1	H	424/433 (97%)	-0.24	2 (0%) 87 89	12, 28, 42, 77	2 (0%)
All	All	3383/3464 (97%)	-0.10	31 (0%) 81 83	12, 30, 48, 84	26 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	425	VAL	5.2
1	D	1	MET	4.7
1	G	425	VAL	4.5
1	F	2	GLU	3.9
1	G	3	GLU	3.6

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

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	LLP	A	209	24/25	0.98	0.05	24,28,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	C	209	24/25	0.98	0.06	22,25,29,29	0
1	LLP	E	209	24/25	0.98	0.05	24,29,32,33	0
1	LLP	F	209	24/25	0.98	0.07	29,33,36,39	0
1	LLP	H	209	24/25	0.98	0.06	22,26,30,32	0
1	LLP	D	209	24/25	0.99	0.05	24,27,32,33	0
1	LLP	G	209	24/25	0.99	0.04	21,25,28,28	0
1	LLP	B	209	24/25	0.99	0.05	21,25,28,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AE3	E	503	9/9	0.74	0.24	55,62,71,72	0
3	NA	G	503	1/1	0.77	0.13	47,47,47,47	1
5	ETE	E	502	14/14	0.77	0.21	55,72,82,83	0
4	AE3	D	502	9/9	0.78	0.27	57,72,83,84	0
6	1PE	H	502	16/16	0.83	0.18	48,66,69,72	0
6	1PE	H	503	16/16	0.83	0.19	54,63,80,81	0
3	NA	C	503	1/1	0.85	0.14	49,49,49,49	0
3	NA	D	504	1/1	0.87	0.11	51,51,51,51	0
3	NA	A	503	1/1	0.88	0.13	55,55,55,55	0
3	NA	B	503	1/1	0.89	0.12	56,56,56,56	0
3	NA	A	502	1/1	0.91	0.12	50,50,50,50	0
3	NA	G	502	1/1	0.93	0.08	63,63,63,63	0
3	NA	H	504	1/1	0.94	0.16	44,44,44,44	0
3	NA	C	504	1/1	0.95	0.07	45,45,45,45	1
2	MES	A	501	12/12	0.95	0.10	34,37,39,47	0
2	MES	E	501	12/12	0.95	0.12	35,39,42,45	0
2	MES	F	501	12/12	0.95	0.12	38,48,52,53	0
2	MES	H	501	12/12	0.95	0.11	34,37,41,48	0
2	MES	D	501	12/12	0.96	0.09	38,39,44,51	0
2	MES	B	501	12/12	0.96	0.10	30,34,38,43	0
3	NA	B	502	1/1	0.96	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	G	501	12/12	0.97	0.09	28,34,38,44	0
2	MES	C	501	12/12	0.97	0.09	33,35,37,42	0
3	NA	D	503	1/1	0.97	0.13	39,39,39,39	0
3	NA	C	505	1/1	0.98	0.05	51,51,51,51	0
3	NA	C	502	1/1	0.99	0.11	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.