



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:01 PM UTC

PDB ID : 3W1H / pdb_00003w1h
Title : Crystal structure of the selenocysteine synthase SelA from Aquifex aeolicus
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.
Deposited on : 2012-11-15
Resolution : 3.89 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

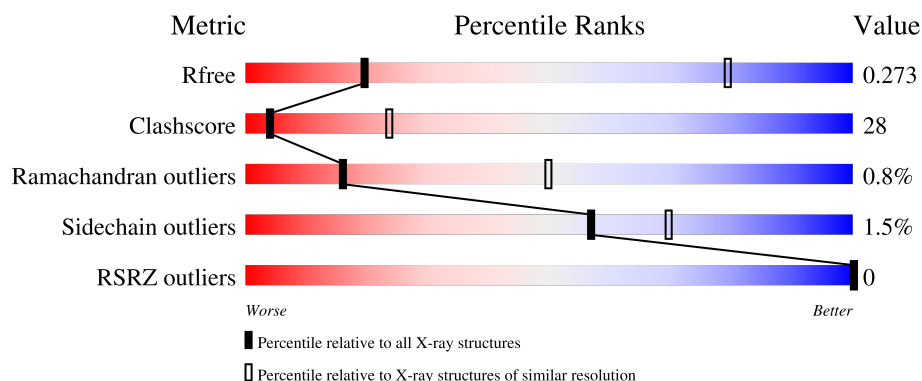
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	452	
1	B	452	
1	C	452	
1	D	452	
1	E	452	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	LLP	B	285	-	-	X	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16913 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 L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	B	443	Total	C	N	O	P	S	0	0	0
			3501	2230	606	654	1	10			
1	C	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	D	395	Total	C	N	O	P	S	0	0	0
			3115	1980	542	582	1	10			
1	E	399	Total	C	N	O	P	S	0	0	0
			3147	2000	546	590	1	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	engineered mutation	UNP O67140
A	21	ALA	LYS	engineered mutation	UNP O67140
A	46	ALA	LYS	engineered mutation	UNP O67140
A	48	ALA	LYS	engineered mutation	UNP O67140
B	19	ALA	LYS	engineered mutation	UNP O67140
B	21	ALA	LYS	engineered mutation	UNP O67140
B	46	ALA	LYS	engineered mutation	UNP O67140
B	48	ALA	LYS	engineered mutation	UNP O67140
C	19	ALA	LYS	engineered mutation	UNP O67140
C	21	ALA	LYS	engineered mutation	UNP O67140
C	46	ALA	LYS	engineered mutation	UNP O67140
C	48	ALA	LYS	engineered mutation	UNP O67140
D	19	ALA	LYS	engineered mutation	UNP O67140
D	21	ALA	LYS	engineered mutation	UNP O67140
D	46	ALA	LYS	engineered mutation	UNP O67140
D	48	ALA	LYS	engineered mutation	UNP O67140
E	19	ALA	LYS	engineered mutation	UNP O67140
E	21	ALA	LYS	engineered mutation	UNP O67140
E	46	ALA	LYS	engineered mutation	UNP O67140

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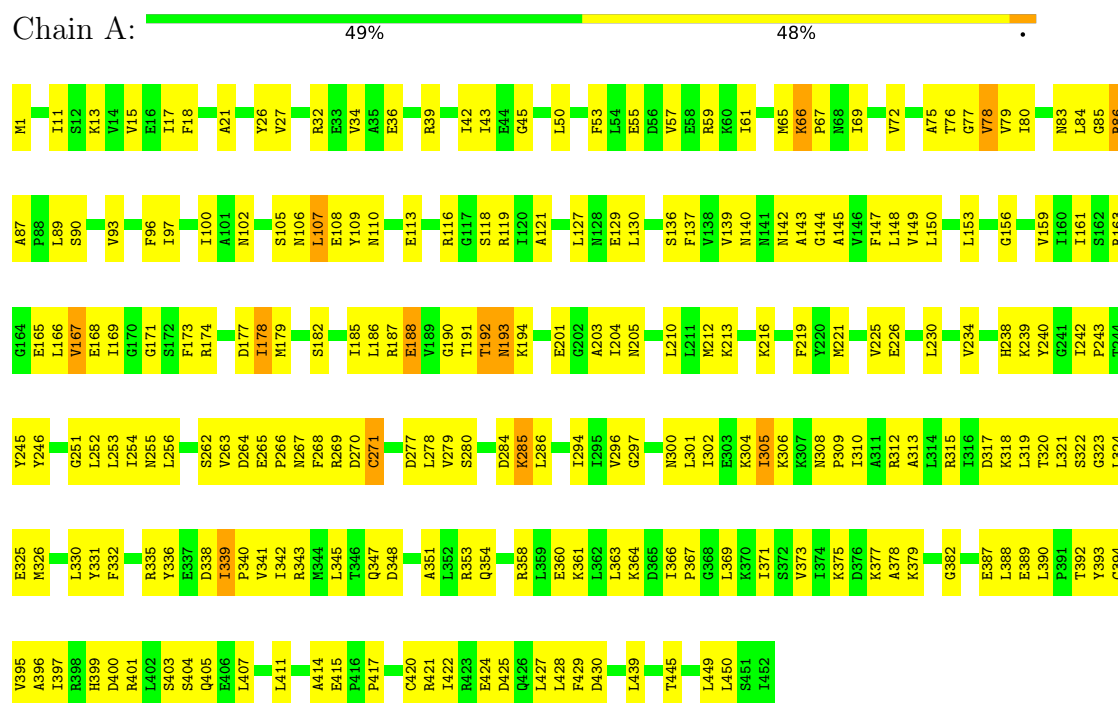
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Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	engineered mutation	UNP O67140

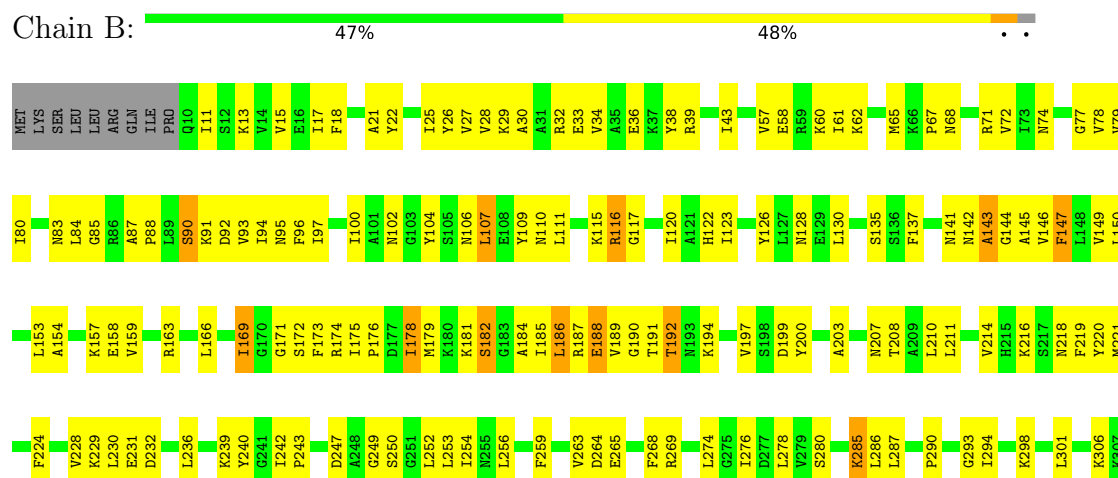
3 Residue-property plots

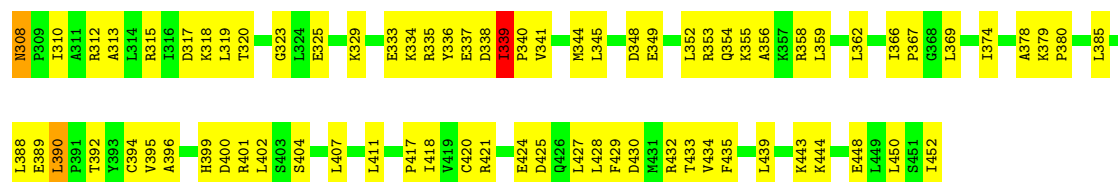
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: L-seryl-tRNA(Sec) selenium transferase



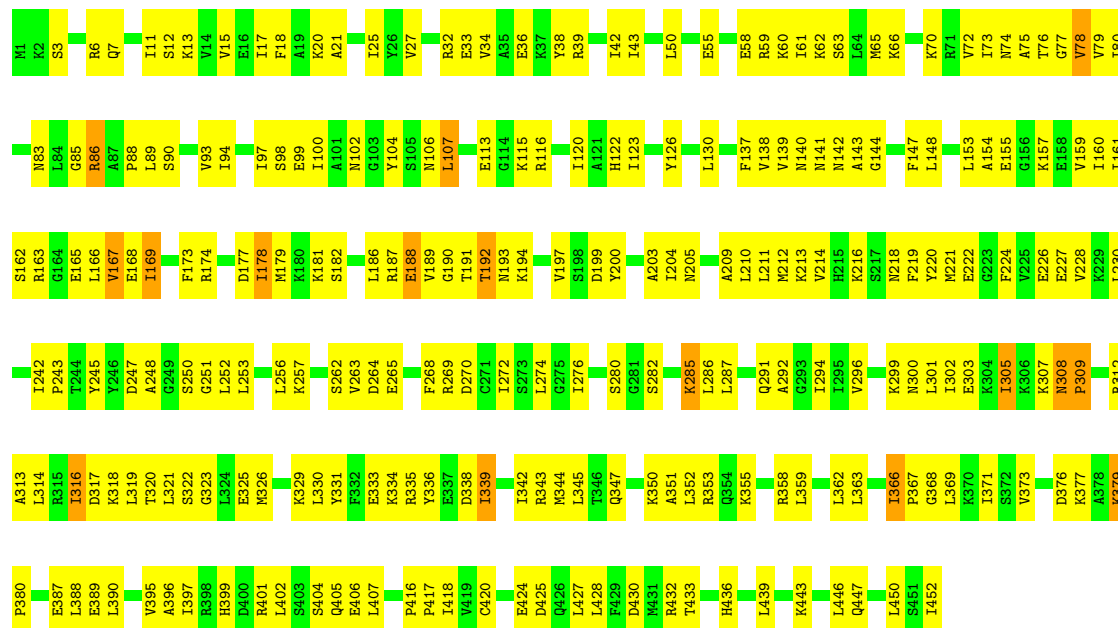
- Molecule 1: L-seryl-tRNA(Sec) selenium transferase





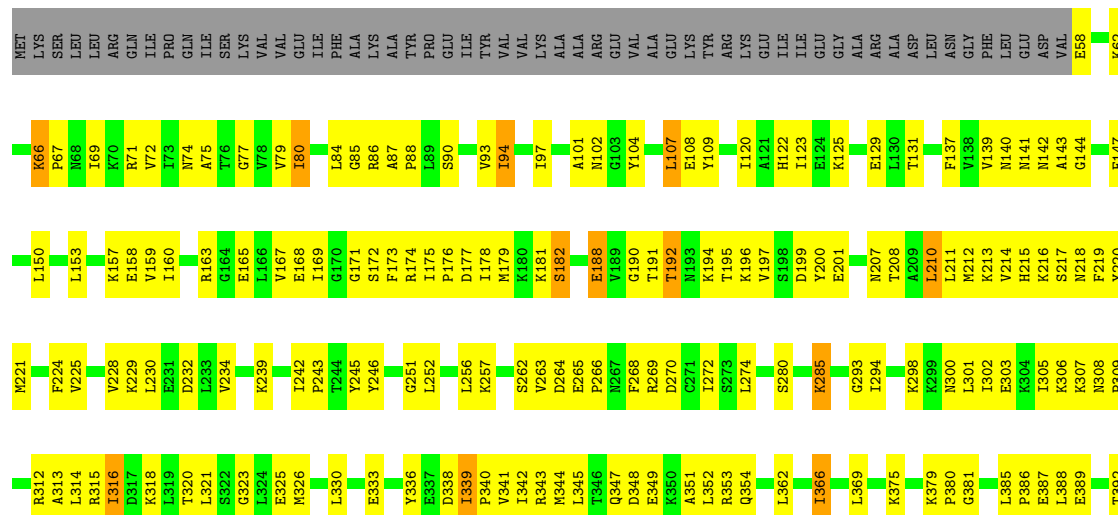
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain C: 46% 51%



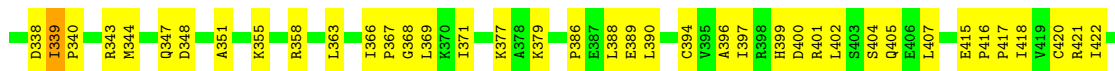
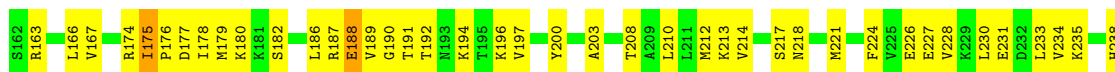
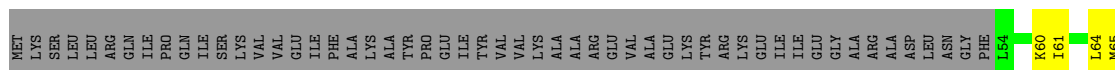
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain D: 44% 41% 13%





• Molecule 1: L-seryl-tRNA(Sec) selenium transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.03Å 167.03Å 211.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.89 49.25 – 3.89	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.25-3.89) 94.1 (49.25-3.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.282 0.203 , 0.273	Depositor DCC
R_{free} test set	1345 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	130.3	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 152.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16913	wwPDB-VP
Average B, all atoms (Å ²)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: LLP

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	0.52	0/3597	0.98	11/4831 (0.2%)
1	B	0.57	0/3522	0.98	12/4731 (0.3%)
1	C	0.53	0/3597	0.96	12/4831 (0.2%)
1	D	0.51	0/3130	0.98	12/4203 (0.3%)
1	E	0.53	0/3162	0.97	10/4247 (0.2%)
All	All	0.53	0/17008	0.97	57/22843 (0.2%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	339	ILE	CA-C-N	9.06	128.66	119.24
1	E	339	ILE	C-N-CA	9.06	128.66	119.24
1	D	308	ASN	CA-C-N	8.96	128.60	119.82
1	D	308	ASN	C-N-CA	8.96	128.60	119.82
1	D	66	LYS	CA-C-N	8.87	128.89	119.76

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	3575	0	3759	228	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3501	0	3668	252	0
1	C	3575	0	3759	236	0
1	D	3115	0	3271	191	0
1	E	3147	0	3301	151	0
All	All	16913	0	17758	963	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 28.

The worst 5 of 963 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:C:102:ASN:HB3	1:D:71:ARG:HH22	1.16	1.03
1:B:72:VAL:HG22	1:B:417:PRO:HG2	1.41	1.03
1:E:123:ILE:HD13	1:E:324:LEU:HD23	1.37	1.02
1:A:69:ILE:HG22	1:B:100:ILE:HD12	1.49	0.95
1:E:254:ILE:HD11	1:E:259:PHE:HE2	1.31	0.94

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	449/452 (99%)	417 (93%)	29 (6%)	3 (1%)	18	53
1	B	440/452 (97%)	403 (92%)	31 (7%)	6 (1%)	9	38
1	C	449/452 (99%)	409 (91%)	36 (8%)	4 (1%)	14	47
1	D	392/452 (87%)	366 (93%)	22 (6%)	4 (1%)	12	45
1	E	396/452 (88%)	374 (94%)	22 (6%)	0	100	100
All	All	2126/2260 (94%)	1969 (93%)	140 (7%)	17 (1%)	16	50

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	B	107	LEU
1	C	192	THR
1	A	107	LEU
1	A	192	THR

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	390/390 (100%)	382 (98%)	8 (2%)	47	65
1	B	381/390 (98%)	375 (98%)	6 (2%)	55	69
1	C	390/390 (100%)	384 (98%)	6 (2%)	57	70
1	D	342/390 (88%)	337 (98%)	5 (2%)	57	70
1	E	346/390 (89%)	343 (99%)	3 (1%)	70	75
All	All	1849/1950 (95%)	1821 (98%)	28 (2%)	57	70

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	VAL
1	E	188	GLU
1	C	188	GLU
1	D	316	ILE
1	C	178	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	436	HIS
1	E	436	HIS
1	D	238	HIS
1	E	300	ASN

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Mol	Chain	Res	Type
1	D	140	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	A	285	1	23,24,25	1.61	6 (26%)	25,32,34	1.54	2 (8%)
1	LLP	D	285	1	23,24,25	1.65	6 (26%)	25,32,34	1.47	2 (8%)
1	LLP	B	285	1	23,24,25	1.57	6 (26%)	25,32,34	1.44	3 (12%)
1	LLP	C	285	1	23,24,25	1.59	4 (17%)	25,32,34	1.52	2 (8%)
1	LLP	E	285	1	23,24,25	1.70	4 (17%)	25,32,34	1.45	3 (12%)

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	A	285	1	-	5/16/17/19	0/1/1/1
1	LLP	D	285	1	-	5/16/17/19	0/1/1/1
1	LLP	B	285	1	-	6/16/17/19	0/1/1/1
1	LLP	C	285	1	-	5/16/17/19	0/1/1/1
1	LLP	E	285	1	-	4/16/17/19	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LLP	C2'-C2	3.78	1.56	1.50
1	E	285	LLP	C4-C4'	3.70	1.54	1.46
1	C	285	LLP	C2'-C2	3.51	1.55	1.50
1	D	285	LLP	C2'-C2	3.44	1.55	1.50
1	E	285	LLP	C2'-C2	3.41	1.55	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LLP	OP4-C5'-C5	6.20	120.98	109.36
1	D	285	LLP	OP4-C5'-C5	5.48	119.63	109.36
1	A	285	LLP	OP4-C5'-C5	5.29	119.26	109.36
1	E	285	LLP	OP4-C5'-C5	4.76	118.27	109.36
1	B	285	LLP	OP4-C5'-C5	4.15	117.13	109.36

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285	LLP	C4-C5-C5'-OP4
1	A	285	LLP	C6-C5-C5'-OP4
1	A	285	LLP	C-CA-CB-CG
1	A	285	LLP	O-C-CA-CB
1	B	285	LLP	C4-C5-C5'-OP4

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	2	0
1	D	285	LLP	3	0
1	B	285	LLP	10	0
1	C	285	LLP	4	0
1	E	285	LLP	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	451/452 (99%)	-0.82	0 100 100	127, 198, 298, 335	0
1	B	442/452 (97%)	-0.79	0 100 100	120, 186, 310, 350	0
1	C	451/452 (99%)	-0.83	0 100 100	122, 198, 299, 337	0
1	D	394/452 (87%)	-0.83	0 100 100	134, 192, 274, 309	0
1	E	398/452 (88%)	-0.81	0 100 100	156, 222, 312, 372	0
All	All	2136/2260 (94%)	-0.82	0 100 100	120, 199, 301, 372	0

There are no RSRZ outliers to report.

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	C	285	24/25	0.97	0.07	113,163,182,192	0
1	LLP	D	285	24/25	0.97	0.06	146,165,183,193	0
1	LLP	E	285	24/25	0.97	0.05	176,200,215,225	0
1	LLP	B	285	24/25	0.98	0.06	123,153,174,176	0
1	LLP	A	285	24/25	0.98	0.05	136,182,191,202	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.