



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2020 – 12:16 PM JST

PDB ID : 6LUT
Title : Crystal structure of Serine Racemase from Dictyostelium discoideum.
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Deposited on : 2020-01-31
Resolution : 1.35 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 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 : 2.14.6
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) : 2.14.6

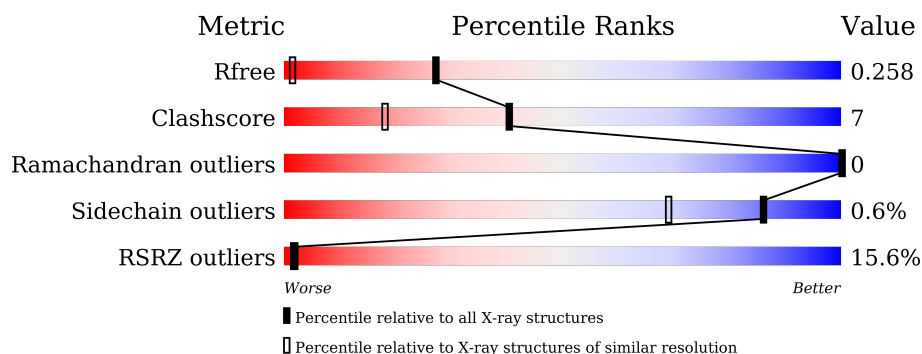
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 on 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	329	<div> <div>12%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	B	329	<div> <div>16%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5091 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 Probable serine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	P	S	0	3	0
			2296	1451	385	445	1	14			
1	B	304	Total	C	N	O	P	S	0	2	0
			2261	1430	380	436	1	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	HIS	-	expression tag	UNP Q54HH2
A	326	HIS	-	expression tag	UNP Q54HH2
A	327	HIS	-	expression tag	UNP Q54HH2
A	328	HIS	-	expression tag	UNP Q54HH2
A	329	HIS	-	expression tag	UNP Q54HH2
B	325	HIS	-	expression tag	UNP Q54HH2
B	326	HIS	-	expression tag	UNP Q54HH2
B	327	HIS	-	expression tag	UNP Q54HH2
B	328	HIS	-	expression tag	UNP Q54HH2
B	329	HIS	-	expression tag	UNP Q54HH2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	271	Total	O	0	0
			271	271		
2	B	263	Total	O	0	0
			263	263		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.64Å 58.07Å 64.53Å 87.40° 72.75° 69.60°	Depositor
Resolution (Å)	36.75 – 1.35 35.92 – 1.35	Depositor EDS
% Data completeness (in resolution range)	94.4 (36.75-1.35) 89.2 (35.92-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.248 , 0.268 0.252 , 0.258	Depositor DCC
R_{free} test set	5239 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 24.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.257 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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

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	0.39	0/2309	0.61	0/3126
1	B	0.39	0/2270	0.61	0/3072
All	All	0.39	0/4579	0.61	0/6198

There are no bond length outliers.

There are no bond angle outliers.

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	2296	0	2323	36	0
1	B	2261	0	2287	30	0
2	A	271	0	0	10	0
2	B	263	0	0	8	0
All	All	5091	0	4610	66	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 7.

All (66) 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:165:LEU:HB2	2:B:404:HOH:O	1.56	1.04
1:A:26:THR:HG23	2:A:407:HOH:O	1.64	0.97
1:B:167:LEU:HD22	2:B:434:HOH:O	1.67	0.94
1:A:309:ILE:HG12	2:A:402:HOH:O	1.69	0.92
1:A:24:HIS:HB2	2:A:407:HOH:O	1.72	0.90
1:A:57:MET:SD	2:A:535:HOH:O	2.37	0.82
1:A:26:THR:CG2	2:A:407:HOH:O	2.25	0.75
1:B:12:ILE:CG2	2:B:404:HOH:O	2.34	0.75
1:B:12:ILE:HG21	2:B:404:HOH:O	1.86	0.75
1:A:50:GLN:HA	2:A:407:HOH:O	1.87	0.75
1:B:65:PHE:CE1	2:B:401:HOH:O	2.46	0.69
1:A:87:ALA:HA	2:A:535:HOH:O	1.97	0.63
1:B:167:LEU:CD2	2:B:434:HOH:O	2.37	0.62
1:A:194:ALA:HB1	1:A:201:ILE:HG21	1.85	0.58
1:B:12:ILE:HG22	2:B:404:HOH:O	2.03	0.56
1:B:194:ALA:HB1	1:B:201:ILE:HG21	1.87	0.55
1:A:202:LYS:HB3	1:A:204:PHE:CE2	2.43	0.54
1:A:291:ILE:HD12	1:A:307:ILE:HD11	1.89	0.52
1:B:65:PHE:HE1	2:B:401:HOH:O	1.90	0.52
1:A:81:SER:HB3	1:A:103:VAL:HG11	1.93	0.50
1:B:156:VAL:O	1:B:160:GLN:HG2	2.11	0.50
1:B:81:SER:HB3	1:B:103:VAL:HG11	1.93	0.49
1:B:47:GLU:HB2	1:B:309:ILE:O	2.12	0.49
1:B:56:LLP:H2'1	1:B:83:ASN:ND2	2.28	0.49
1:A:75:GLY:HA2	1:A:97:VAL:HG13	1.94	0.49
1:A:47:GLU:HB2	1:A:309:ILE:O	2.14	0.48
1:A:23:ILE:HG22	1:A:57:MET:HG3	1.96	0.48
1:B:187:LEU:HD22	1:B:205:ALA:HB2	1.95	0.47
1:B:23:ILE:HG22	1:B:57:MET:HG3	1.97	0.47
1:B:176:ALA:HA	1:B:202:LYS:O	2.15	0.47
1:A:56:LLP:H2'1	1:A:83:ASN:ND2	2.30	0.47
1:A:181:VAL:HG21	1:A:214:THR:HG21	1.98	0.45
1:B:55:PHE:CE2	1:B:186:LEU:HB2	2.52	0.45
1:B:57:MET:HA	1:B:87:ALA:HB1	1.98	0.45
1:A:176:ALA:HA	1:A:202:LYS:O	2.17	0.44
1:A:167:LEU:HD21	1:A:306:GLY:HA3	1.99	0.44
1:A:175:ASP:HB2	1:A:302:ILE:HG23	1.99	0.44
1:B:75:GLY:HA2	1:B:97:VAL:HG13	1.99	0.44
1:A:187:LEU:HD22	1:A:205:ALA:HB2	2.00	0.43
1:B:55:PHE:CZ	1:B:56:LLP:HE2	2.54	0.43
1:A:55:PHE:CE2	1:A:186:LEU:HB2	2.53	0.43
1:A:205:ALA:HB3	1:A:257:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:VAL:HG21	1:B:214:THR:HG21	1.99	0.43
1:B:149:HIS:HE1	1:B:151:PHE:CZ	2.36	0.43
1:B:60:ALA:HB1	1:B:88:LEU:HA	2.00	0.43
1:A:291:ILE:CD1	1:A:305:VAL:HG11	2.49	0.43
1:B:205:ALA:HB3	1:B:257:VAL:HG22	2.00	0.43
1:B:167:LEU:HD21	1:B:306:GLY:HA3	2.01	0.42
1:B:56:LLP:H2'1	1:B:83:ASN:HD22	1.85	0.42
1:A:52:THR:CG2	2:A:535:HOH:O	2.66	0.42
1:A:156:VAL:O	1:A:160:GLN:HG2	2.19	0.42
1:A:52:THR:HG21	2:A:535:HOH:O	2.19	0.42
1:A:149:HIS:HE1	1:A:151:PHE:CZ	2.38	0.41
1:A:101:VAL:HG11	1:A:115:ILE:HD13	2.02	0.41
1:B:101:VAL:HG11	1:B:115:ILE:HD13	2.02	0.41
1:B:77:VAL:HA	1:B:100:TYR:O	2.20	0.41
1:A:77:VAL:HA	1:A:100:TYR:O	2.20	0.41
1:A:34:ILE:HG22	1:A:42:LEU:HD12	2.03	0.41
1:A:57:MET:CE	1:A:61[B]:CYS:SG	3.09	0.41
1:A:80:SER:O	1:A:85:GLY:HA3	2.20	0.41
1:B:34:ILE:HG22	1:B:42:LEU:HD12	2.01	0.41
1:A:55:PHE:CZ	1:A:56:LLP:HE2	2.56	0.41
1:A:50:GLN:NE2	2:A:407:HOH:O	2.54	0.40
1:A:60:ALA:HB1	1:A:88:LEU:HA	2.02	0.40
1:B:177:ILE:HA	1:B:306:GLY:O	2.22	0.40
1:A:177:ILE:HA	1:A:306:GLY:O	2.22	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	305/329 (93%)	298 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	299/329 (91%)	295 (99%)	4 (1%)	0	100	100
All	All	604/658 (92%)	593 (98%)	11 (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	247/280 (88%)	245 (99%)	2 (1%)	81	59
1	B	242/280 (86%)	241 (100%)	1 (0%)	91	81
All	All	489/560 (87%)	486 (99%)	3 (1%)	86	69

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ASP
1	A	202	LYS
1	B	234	ILE

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

Mol	Chain	Res	Type
1	B	138	GLN
1	B	142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	B	56	1	23,24,25	2.53	5 (21%)	25,32,34	1.55	4 (16%)
1	LLP	A	56	1	23,24,25	2.52	5 (21%)	25,32,34	1.55	5 (20%)

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	B	56	1	-	5/16/17/19	0/1/1/1
1	LLP	A	56	1	-	5/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	LLP	C3-C2	7.20	1.48	1.40
1	B	56	LLP	C3-C2	7.17	1.48	1.40
1	B	56	LLP	C4'-NZ	5.53	1.45	1.27
1	A	56	LLP	C4'-NZ	5.52	1.45	1.27
1	B	56	LLP	C4-C5	5.44	1.48	1.42
1	A	56	LLP	C4-C5	5.38	1.48	1.42
1	B	56	LLP	C4-C3	4.65	1.47	1.40
1	A	56	LLP	C4-C3	4.51	1.47	1.40
1	A	56	LLP	C4-C4'	2.78	1.51	1.46
1	B	56	LLP	C4-C4'	2.76	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LLP	C4-C3-C2	-3.79	117.84	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	LLP	C4-C3-C2	-3.76	117.86	120.19
1	A	56	LLP	C4-C4'-NZ	-3.28	109.27	124.31
1	B	56	LLP	C4-C4'-NZ	-3.22	109.52	124.31
1	B	56	LLP	C3-C4-C5	-3.15	115.84	118.26
1	A	56	LLP	C6-N1-C2	2.72	124.20	119.17
1	A	56	LLP	C3-C4-C5	-2.68	116.21	118.26
1	B	56	LLP	C6-N1-C2	2.48	123.77	119.17
1	A	56	LLP	O3-C3-C2	2.03	121.91	117.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	56	LLP	C4-C4'-NZ-CE
1	A	56	LLP	C4-C4'-NZ-CE
1	A	56	LLP	CG-CD-CE-NZ
1	B	56	LLP	CG-CD-CE-NZ
1	B	56	LLP	CA-CB-CG-CD
1	A	56	LLP	CA-CB-CG-CD
1	B	56	LLP	CD-CE-NZ-C4'
1	A	56	LLP	CD-CE-NZ-C4'
1	B	56	LLP	C3-C4-C4'-NZ
1	A	56	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	56	LLP	3	0
1	A	56	LLP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	306/329 (93%)	1.18	41 (13%) 3 3	11, 18, 29, 38	0
1	B	303/329 (92%)	1.21	54 (17%) 1 1	11, 18, 30, 39	0
All	All	609/658 (92%)	1.20	95 (15%) 2 2	11, 18, 30, 39	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	6.5
1	A	236	ASP	5.4
1	A	5	ALA	5.1
1	B	127	ALA	5.0
1	B	234	ILE	5.0
1	A	128	THR	4.6
1	A	316	LEU	4.5
1	A	234	ILE	4.4
1	A	209	LEU	4.1
1	B	236	ASP	4.1
1	A	314	VAL	4.0
1	A	105	GLU	4.0
1	A	129	LEU	4.0
1	B	314	VAL	3.9
1	B	5	ALA	3.9
1	B	302	ILE	3.9
1	B	215	TYR	3.9
1	B	69	GLU	3.8
1	B	219	LEU	3.8
1	B	209	LEU	3.7
1	A	127	ALA	3.6
1	B	128	THR	3.5
1	B	316	LEU	3.5
1	A	267	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	240	THR	3.2
1	B	125	CYS	3.2
1	B	210	GLY	3.1
1	B	22	TYR	3.1
1	A	315	ASP	3.1
1	B	300	LYS	3.1
1	A	226	HIS	3.0
1	A	125	CYS	3.0
1	B	145	CYS	3.0
1	A	232	ASN	3.0
1	B	267	TYR	2.9
1	B	225	LYS	2.9
1	B	245	LEU	2.9
1	A	22	TYR	2.8
1	A	260	VAL	2.8
1	B	259	LEU	2.8
1	B	201	ILE	2.7
1	B	308	ILE	2.7
1	A	131	ALA	2.7
1	A	247	PHE	2.6
1	A	240	THR	2.5
1	A	220	SER	2.5
1	A	108	PRO	2.5
1	A	219	LEU	2.5
1	B	233	THR	2.5
1	B	156	VAL	2.5
1	B	260	VAL	2.5
1	B	177	ILE	2.4
1	A	123	THR	2.4
1	A	139	LEU	2.4
1	B	204	PHE	2.4
1	B	211	ALA	2.3
1	B	265	ILE	2.3
1	B	247	PHE	2.3
1	A	142	GLN	2.3
1	B	315	ASP	2.3
1	B	239	LEU	2.3
1	A	241	THR	2.3
1	B	223	ILE	2.3
1	B	218	LEU	2.3
1	B	241	THR	2.3
1	A	205	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	105	GLU	2.2
1	B	235	ALA	2.2
1	A	134	SER	2.2
1	A	233	THR	2.2
1	B	238	LEU	2.2
1	B	301	ASP	2.2
1	B	217	SER	2.2
1	B	232	ASN	2.2
1	A	67	LEU	2.2
1	A	112	LEU	2.2
1	B	258	ILE	2.2
1	B	131	ALA	2.2
1	B	12	ILE	2.1
1	A	274	GLU	2.1
1	B	205	ALA	2.1
1	B	220	SER	2.1
1	A	103	VAL	2.1
1	A	308	ILE	2.1
1	A	235	ALA	2.1
1	B	112	LEU	2.1
1	B	139	LEU	2.1
1	A	257	VAL	2.1
1	A	69	GLU	2.0
1	B	296	PHE	2.0
1	B	271	LEU	2.0
1	B	213	ASP	2.0
1	A	64	ILE	2.0
1	B	192	ILE	2.0
1	A	295	GLU	2.0

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(\AA^2)	Q<0.9
1	LLP	B	56	24/25	0.93	0.13	11,15,17,18	0
1	LLP	A	56	24/25	0.93	0.12	11,15,17,18	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.