



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:11 PM UTC

PDB ID : 8SRU / pdb_00008sru
Title : Crystal structure of O-acetyl-L-serine sulfhydrylase A (CysK) from Staphylococcus aureus NCTC 8325 complexed with a serine acetyltransferase (CysE) derived peptide
Authors : Pederick, J.L.; Vandborg, B.C.; Bruning, J.B.
Deposited on : 2023-05-07
Resolution : 1.50 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 : 4-5-2 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

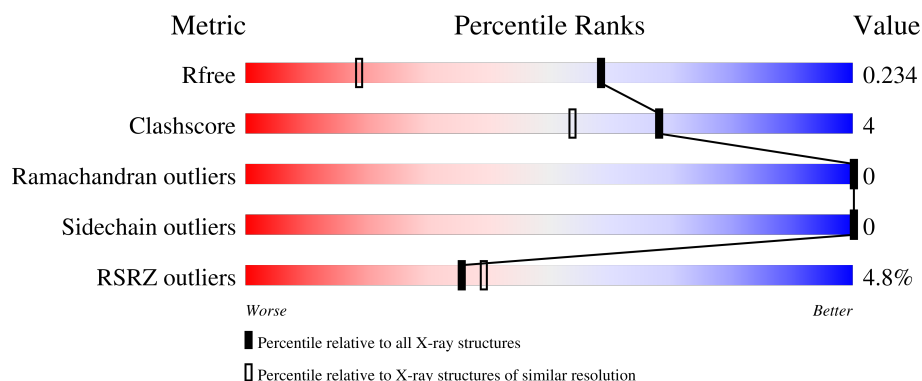
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	318	4% 92% • •
1	B	318	4% 90% 8% •
1	C	318	5% 89% 7% •
1	D	318	5% 92% 7% •
2	E	10	30% 10% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	10	 40% 60%
2	G	10	 30% 10% 60%
2	H	10	 40% 60%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10426 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 Cysteine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	P	S	0	1	0
			2272	1439	381	444	1	7			
1	B	313	Total	C	N	O	P	S	0	0	0
			2313	1461	396	447	1	8			
1	C	306	Total	C	N	O	P	S	0	0	0
			2268	1440	381	438	1	8			
1	D	312	Total	C	N	O	P	S	0	1	0
			2332	1475	397	451	1	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q2G0Q8
A	-6	GLY	-	expression tag	UNP Q2G0Q8
A	-5	HIS	-	expression tag	UNP Q2G0Q8
A	-4	HIS	-	expression tag	UNP Q2G0Q8
A	-3	HIS	-	expression tag	UNP Q2G0Q8
A	-2	HIS	-	expression tag	UNP Q2G0Q8
A	-1	HIS	-	expression tag	UNP Q2G0Q8
A	0	HIS	-	expression tag	UNP Q2G0Q8
B	-7	MET	-	expression tag	UNP Q2G0Q8
B	-6	GLY	-	expression tag	UNP Q2G0Q8
B	-5	HIS	-	expression tag	UNP Q2G0Q8
B	-4	HIS	-	expression tag	UNP Q2G0Q8
B	-3	HIS	-	expression tag	UNP Q2G0Q8
B	-2	HIS	-	expression tag	UNP Q2G0Q8
B	-1	HIS	-	expression tag	UNP Q2G0Q8
B	0	HIS	-	expression tag	UNP Q2G0Q8
C	-7	MET	-	expression tag	UNP Q2G0Q8
C	-6	GLY	-	expression tag	UNP Q2G0Q8
C	-5	HIS	-	expression tag	UNP Q2G0Q8
C	-4	HIS	-	expression tag	UNP Q2G0Q8
C	-3	HIS	-	expression tag	UNP Q2G0Q8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q2G0Q8
C	-1	HIS	-	expression tag	UNP Q2G0Q8
C	0	HIS	-	expression tag	UNP Q2G0Q8
D	-7	MET	-	expression tag	UNP Q2G0Q8
D	-6	GLY	-	expression tag	UNP Q2G0Q8
D	-5	HIS	-	expression tag	UNP Q2G0Q8
D	-4	HIS	-	expression tag	UNP Q2G0Q8
D	-3	HIS	-	expression tag	UNP Q2G0Q8
D	-2	HIS	-	expression tag	UNP Q2G0Q8
D	-1	HIS	-	expression tag	UNP Q2G0Q8
D	0	HIS	-	expression tag	UNP Q2G0Q8

- Molecule 2 is a protein called Serine acetyltransferase (CysE) derived peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	4	Total	C	N	O	0	0	0
			37	25	4	8			
2	E	4	Total	C	N	O	0	0	0
			37	25	4	8			
2	F	4	Total	C	N	O	0	0	0
			37	25	4	8			
2	G	4	Total	C	N	O	0	0	0
			37	25	4	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	245	Total	O	0	0
			245	245		
3	B	255	Total	O	0	0
			255	255		
3	C	285	Total	O	0	0
			285	285		
3	D	275	Total	O	0	0
			275	275		
3	H	9	Total	O	0	0
			9	9		
3	E	8	Total	O	0	0
			8	8		
3	F	7	Total	O	0	0
			7	7		
3	G	9	Total	O	0	0
			9	9		

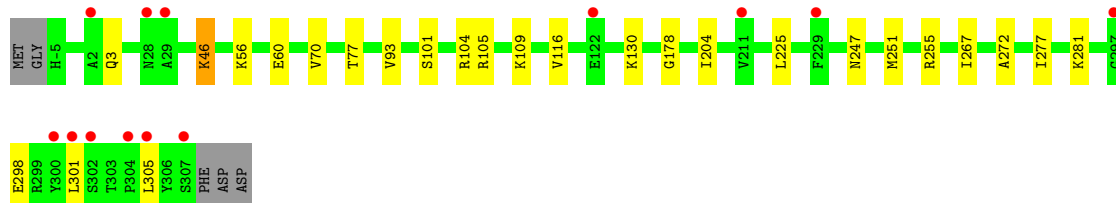
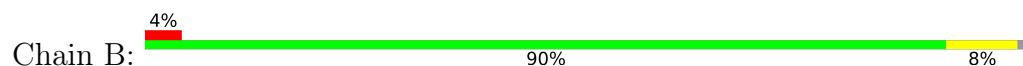
3 Residue-property plots [i](#)

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.

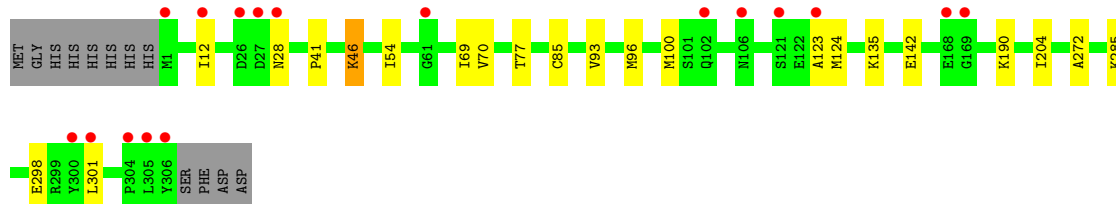
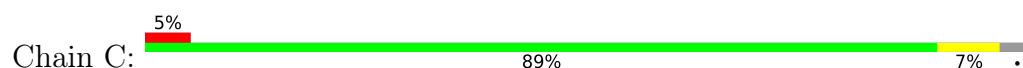
- Molecule 1: Cysteine synthase



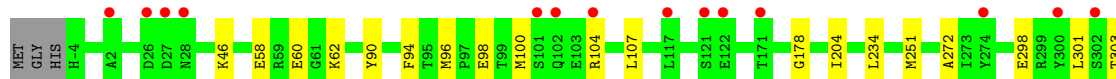
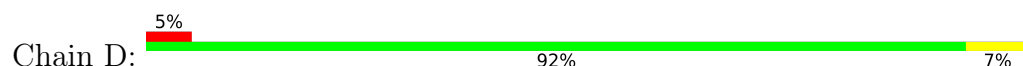
- Molecule 1: Cysteine synthase

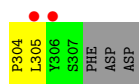


- Molecule 1: Cysteine synthase



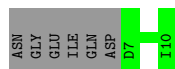
- Molecule 1: Cysteine synthase





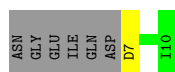
- Molecule 2: Serine acetyltransferase (CysE) derived peptide

Chain H: 



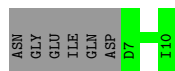
- Molecule 2: Serine acetyltransferase (CysE) derived peptide

Chain E: 



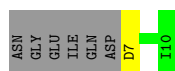
- Molecule 2: Serine acetyltransferase (CysE) derived peptide

Chain F: 



- Molecule 2: Serine acetyltransferase (CysE) derived peptide

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.66Å 96.74Å 94.29Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	39.05 – 1.50 39.05 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.05-1.50) 95.2 (39.05-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.185 , 0.219 (Not available) , 0.234	Depositor DCC
R_{free} test set	9661 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10426	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0603e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.71	0/2285	0.82	0/3094
1	B	0.69	0/2331	0.79	0/3162
1	C	0.80	0/2281	0.84	0/3087
1	D	0.74	0/2350	0.84	0/3182
2	E	0.78	0/37	0.78	0/48
2	F	0.72	0/37	0.72	0/48
2	G	0.83	0/37	0.95	0/48
2	H	0.84	0/37	0.81	0/48
All	All	0.74	0/9395	0.82	0/12717

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 [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	2272	0	2284	9	0
1	B	2313	0	2292	21	0
1	C	2268	0	2293	19	0
1	D	2332	0	2334	20	0
2	E	37	0	34	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	37	0	34	0	0
2	G	37	0	34	2	0
2	H	37	0	34	0	0
3	A	245	0	0	1	0
3	B	255	0	0	4	0
3	C	285	0	0	1	0
3	D	275	0	0	5	0
3	E	8	0	0	0	0
3	F	7	0	0	0	0
3	G	9	0	0	0	0
3	H	9	0	0	0	0
All	All	10426	0	9339	67	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 (67) 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:D:305:LEU:HA	3:D:477:HOH:O	1.71	0.89
1:D:298:GLU:HA	1:D:301:LEU:CD1	2.10	0.82
1:D:298:GLU:HA	1:D:301:LEU:HD13	1.66	0.76
1:D:251:MET:HB3	3:D:477:HOH:O	1.93	0.68
1:C:298:GLU:HA	1:C:301:LEU:CD1	2.23	0.68
1:A:123:ALA:HB1	2:E:7:ASP:HB2	1.77	0.66
1:D:94:PHE:HB2	1:D:96:MET:HE1	1.79	0.64
1:B:298:GLU:HA	1:B:301:LEU:HD11	1.78	0.64
1:D:100:MET:HE3	1:D:104:ARG:HG3	1.79	0.63
1:C:12:ILE:HG13	1:C:41:PRO:HG3	1.82	0.62
1:C:123:ALA:HB1	2:G:7:ASP:HB2	1.81	0.61
1:B:298:GLU:HA	1:B:301:LEU:CD1	2.31	0.61
1:C:298:GLU:HA	1:C:301:LEU:HD11	1.83	0.60
1:C:190:LYS:NZ	3:C:402:HOH:O	2.33	0.60
1:C:96:MET:HG3	1:C:100:MET:CE	2.32	0.60
1:D:303:THR:HB	1:D:304:PRO:HD2	1.85	0.59
1:B:104:ARG:NH2	3:B:401:HOH:O	2.36	0.58
1:B:104:ARG:NH1	3:B:402:HOH:O	2.38	0.56
1:D:204:ILE:HD13	1:D:272:ALA:HA	1.87	0.55
1:A:12:ILE:HD11	1:A:41:PRO:HB3	1.89	0.55
1:A:204:ILE:HD13	1:A:272:ALA:HA	1.89	0.55
1:B:204:ILE:HD13	1:B:272:ALA:HA	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LEU:HD12	3:D:477:HOH:O	2.07	0.54
1:D:60:GLU:OE1	1:D:62:LYS:NZ	2.39	0.53
1:B:46:LLP:HE3	1:B:77:THR:OG1	2.08	0.53
1:C:28:ASN:HA	1:C:285:LYS:HD2	1.92	0.52
1:B:104:ARG:NH2	3:B:403:HOH:O	2.40	0.52
1:C:298:GLU:HA	1:C:301:LEU:HD13	1.92	0.52
1:D:94:PHE:CB	1:D:96:MET:HE1	2.40	0.52
1:B:267:ILE:HG13	1:B:305:LEU:HD22	1.93	0.51
1:D:298:GLU:HA	1:D:301:LEU:HD11	1.90	0.50
1:B:116:VAL:HG11	1:B:130:LYS:HE2	1.94	0.50
1:D:96:MET:HG3	1:D:100:MET:SD	2.51	0.50
1:C:204:ILE:HD13	1:C:272:ALA:HA	1.93	0.50
1:B:277:ILE:HG22	1:B:281:LYS:HE2	1.95	0.48
1:C:96:MET:HG3	1:C:100:MET:HE3	1.94	0.48
1:B:56:LYS:HE2	1:B:60:GLU:OE2	2.12	0.48
1:B:298:GLU:O	1:B:301:LEU:HD13	2.14	0.48
1:D:178:GLY:HA2	1:D:204:ILE:HB	1.96	0.47
1:A:12:ILE:HG13	1:A:41:PRO:HG3	1.97	0.47
1:B:101:SER:O	1:B:105:ARG:HG3	2.15	0.47
1:B:105:ARG:O	1:B:109:LYS:HG3	2.15	0.47
1:B:251:MET:HE3	1:B:255:ARG:NH2	2.31	0.46
1:D:62:LYS:HE2	3:D:637:HOH:O	2.16	0.46
1:A:59:ARG:HD3	1:D:98:GLU:HB2	1.98	0.45
1:A:104:ARG:HA	1:A:104:ARG:HD3	1.73	0.44
1:D:58:GLU:HG2	1:D:90:TYR:OH	2.18	0.44
1:A:104:ARG:NH1	3:A:413:HOH:O	2.51	0.43
1:A:94:PHE:HB2	1:A:96:MET:HE1	2.00	0.43
1:B:70:VAL:HA	1:B:93:VAL:O	2.18	0.43
1:C:12:ILE:HD11	1:C:41:PRO:HB3	2.01	0.43
1:D:234:LEU:O	3:D:401:HOH:O	2.21	0.43
1:C:54:ILE:HD11	1:C:69:ILE:HD13	2.01	0.42
1:C:301:LEU:HD21	1:D:107:LEU:HB2	2.02	0.42
1:B:247:ASN:O	1:B:251:MET:HG3	2.19	0.42
1:C:70:VAL:HA	1:C:93:VAL:O	2.19	0.42
1:C:46:LLP:HE3	1:C:77:THR:OG1	2.20	0.42
1:D:298:GLU:O	1:D:301:LEU:HD13	2.19	0.41
1:C:100:MET:HE3	1:C:100:MET:HB2	1.62	0.41
1:C:124:MET:HB2	2:G:7:ASP:OD2	2.20	0.41
1:A:70:VAL:HA	1:A:93:VAL:O	2.21	0.41
1:B:178:GLY:HA2	1:B:204:ILE:HB	2.03	0.41
1:C:135:LYS:HD2	1:C:142:GLU:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:HG3	3:B:505:HOH:O	2.20	0.40
1:C:69:ILE:HD11	1:C:85:CYS:SG	2.61	0.40
1:B:298:GLU:C	1:B:301:LEU:HD13	2.46	0.40
1:B:46:LLP:H6	1:B:225:LEU:HD21	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	303/318 (95%)	296 (98%)	7 (2%)	0	100	100
1	B	310/318 (98%)	303 (98%)	7 (2%)	0	100	100
1	C	303/318 (95%)	295 (97%)	8 (3%)	0	100	100
1	D	310/318 (98%)	302 (97%)	8 (3%)	0	100	100
2	E	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
2	F	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
2	G	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
2	H	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
All	All	1234/1312 (94%)	1200 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	232/251 (92%)	232 (100%)	0	100	100
1	B	234/251 (93%)	234 (100%)	0	100	100
1	C	230/251 (92%)	230 (100%)	0	100	100
1	D	239/251 (95%)	239 (100%)	0	100	100
2	E	4/9 (44%)	4 (100%)	0	100	100
2	F	4/9 (44%)	4 (100%)	0	100	100
2	G	4/9 (44%)	4 (100%)	0	100	100
2	H	4/9 (44%)	4 (100%)	0	100	100
All	All	951/1040 (91%)	951 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	102	GLN
1	A	144	GLN
1	A	145	GLN
1	B	-1	HIS
1	B	11	GLN
1	B	23	ASN
1	C	11	GLN
1	C	138	HIS
1	D	-4	HIS
1	D	11	GLN
1	D	165	GLN
1	D	278	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	46	1	23,24,25	2.31	8 (34%)	25,32,34	1.60	4 (16%)
1	LLP	D	46	1	23,24,25	2.42	8 (34%)	25,32,34	1.51	6 (24%)
1	LLP	B	46	1	23,24,25	2.34	5 (21%)	25,32,34	1.49	4 (16%)
1	LLP	C	46	1	23,24,25	2.43	8 (34%)	25,32,34	2.22	8 (32%)

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	46	1	-	1/16/17/19	0/1/1/1
1	LLP	D	46	1	-	4/16/17/19	0/1/1/1
1	LLP	B	46	1	-	3/16/17/19	0/1/1/1
1	LLP	C	46	1	-	1/16/17/19	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	LLP	C4-C4'	7.20	1.62	1.46
1	C	46	LLP	C4-C4'	7.06	1.61	1.46
1	D	46	LLP	C4-C4'	6.84	1.61	1.46
1	A	46	LLP	C4-C4'	6.23	1.59	1.46
1	D	46	LLP	C4-C5	-5.16	1.34	1.42
1	B	46	LLP	C4'-NZ	4.62	1.42	1.27
1	C	46	LLP	C4-C5	-4.54	1.35	1.42
1	D	46	LLP	C4'-NZ	4.43	1.42	1.27
1	A	46	LLP	C4'-NZ	4.12	1.40	1.27
1	C	46	LLP	C4'-NZ	3.71	1.39	1.27
1	A	46	LLP	C6-N1	3.42	1.41	1.34
1	C	46	LLP	C2'-C2	3.36	1.55	1.50
1	A	46	LLP	C4-C5	-3.17	1.37	1.42
1	B	46	LLP	C6-N1	3.14	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	LLP	C5'-C5	2.99	1.58	1.50
1	C	46	LLP	C6-N1	2.99	1.40	1.34
1	B	46	LLP	C4-C5	-2.95	1.37	1.42
1	A	46	LLP	P-OP3	-2.74	1.44	1.54
1	D	46	LLP	C6-N1	2.72	1.40	1.34
1	A	46	LLP	C3-C2	2.69	1.43	1.41
1	D	46	LLP	C2'-C2	2.66	1.54	1.50
1	C	46	LLP	C3-C2	2.40	1.43	1.41
1	D	46	LLP	C5'-C5	2.40	1.57	1.50
1	A	46	LLP	C2'-C2	2.36	1.54	1.50
1	A	46	LLP	C5'-C5	2.29	1.56	1.50
1	C	46	LLP	CD-CE	2.24	1.59	1.51
1	D	46	LLP	CE-NZ	2.13	1.51	1.46
1	C	46	LLP	O3-C3	-2.11	1.32	1.36
1	D	46	LLP	CD-CE	2.08	1.58	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	LLP	C4-C3-C2	5.91	123.47	120.14
1	C	46	LLP	C2'-C2-C3	4.60	126.18	120.80
1	A	46	LLP	CE-NZ-C4'	-4.05	105.74	118.72
1	C	46	LLP	OP4-C5'-C5	3.79	116.45	109.36
1	C	46	LLP	CE-NZ-C4'	-3.70	106.86	118.72
1	B	46	LLP	CE-NZ-C4'	-3.67	106.96	118.72
1	A	46	LLP	OP4-C5'-C5	3.29	115.53	109.36
1	D	46	LLP	CE-NZ-C4'	-3.19	108.49	118.72
1	C	46	LLP	C3-C2-N1	-3.17	116.97	120.96
1	B	46	LLP	C2'-C2-C3	3.08	124.40	120.80
1	D	46	LLP	C4-C3-C2	2.96	121.81	120.14
1	C	46	LLP	C4-C4'-NZ	-2.67	111.74	124.04
1	D	46	LLP	C2'-C2-C3	2.62	123.87	120.80
1	D	46	LLP	OP4-C5'-C5	2.62	114.27	109.36
1	A	46	LLP	C2'-C2-C3	2.61	123.85	120.80
1	B	46	LLP	C5-C6-N1	-2.47	119.82	123.83
1	D	46	LLP	C5-C6-N1	-2.34	120.02	123.83
1	A	46	LLP	C5-C6-N1	-2.19	120.28	123.83
1	B	46	LLP	C5'-C5-C6	-2.10	115.93	119.36
1	C	46	LLP	C3-C4-C4'	2.08	124.15	120.40
1	D	46	LLP	C5'-C5-C6	-2.06	116.00	119.36
1	C	46	LLP	C5-C4-C4'	-2.01	118.37	121.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	46	LLP	C6-C5-C5'-OP4
1	A	46	LLP	CG-CD-CE-NZ
1	D	46	LLP	CG-CD-CE-NZ
1	B	46	LLP	C5'-OP4-P-OP1
1	D	46	LLP	C5'-OP4-P-OP1
1	B	46	LLP	CG-CD-CE-NZ
1	B	46	LLP	CE-CD-CG-CB
1	C	46	LLP	CG-CD-CE-NZ
1	D	46	LLP	C4-C5-C5'-OP4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	46	LLP	2	0
1	C	46	LLP	1	0

5.5 Carbohydrates [i](#)

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	304/318 (95%)	0.51	14 (4%)	37 41	15, 26, 43, 55	1 (0%)
1	B	312/318 (98%)	0.63	13 (4%)	40 44	19, 28, 43, 56	0
1	C	305/318 (95%)	0.37	17 (5%)	30 33	18, 24, 38, 64	0
1	D	311/318 (97%)	0.58	16 (5%)	33 36	15, 28, 44, 67	1 (0%)
2	E	4/10 (40%)	0.41	0	100 100	24, 26, 27, 45	0
2	F	4/10 (40%)	0.76	0	100 100	26, 27, 30, 41	0
2	G	4/10 (40%)	0.67	0	100 100	24, 28, 28, 46	0
2	H	4/10 (40%)	0.62	0	100 100	24, 27, 28, 38	0
All	All	1248/1312 (95%)	0.52	60 (4%)	35 39	15, 26, 43, 67	2 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	ASP	4.4
1	B	305	LEU	4.3
1	C	301	LEU	3.8
1	C	123	ALA	3.4
1	C	26	ASP	3.3
1	B	122	GLU	3.3
1	C	305	LEU	3.1
1	C	28	ASN	3.0
1	C	306	TYR	3.0
1	D	305	LEU	3.0
1	D	306	TYR	3.0
1	C	300	TYR	2.9
1	A	28	ASN	2.9
1	B	307	SER	2.8
1	D	27	ASP	2.8
1	D	26	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	301	LEU	2.7
1	B	302	SER	2.7
1	B	211	VAL	2.7
1	C	1	MET	2.7
1	B	2	ALA	2.6
1	D	28	ASN	2.6
1	C	169	GLY	2.6
1	D	122	GLU	2.5
1	A	283	LEU	2.5
1	D	302	SER	2.5
1	A	27	ASP	2.5
1	D	2	ALA	2.4
1	C	61	GLY	2.4
1	A	25	VAL	2.4
1	A	123	ALA	2.4
1	D	171	THR	2.4
1	B	300	TYR	2.4
1	D	300	TYR	2.4
1	B	28	ASN	2.4
1	B	29	ALA	2.3
1	B	304	PRO	2.3
1	C	304	PRO	2.2
1	A	117	LEU	2.2
1	A	301	LEU	2.2
1	C	168	GLU	2.2
1	A	169	GLY	2.2
1	C	121	SER	2.2
1	D	121	SER	2.2
1	A	26	ASP	2.2
1	A	300	TYR	2.1
1	B	229	PHE	2.1
1	D	102	GLN	2.1
1	C	12	ILE	2.1
1	C	106	ASN	2.1
1	D	117	LEU	2.1
1	A	306	TYR	2.1
1	A	61	GLY	2.1
1	B	297	GLY	2.1
1	A	102	GLN	2.0
1	C	102	GLN	2.0
1	D	274	TYR	2.0
1	D	101	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	104	ARG	2.0
1	A	2	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	B	46	24/25	0.93	0.11	19,22,30,38	0
1	LLP	A	46	24/25	0.96	0.09	17,23,29,32	0
1	LLP	C	46	24/25	0.96	0.09	16,21,29,32	0
1	LLP	D	46	24/25	0.96	0.09	18,23,30,35	0

6.3 Carbohydrates [i](#)

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.