Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 02:19 PM EST

PDB ID	:	1LYL
Title	:	LYSYL-TRNA SYNTHETASE (LYSU) (E.C.6.1.1.6) COMPLEXED WITH LYSINE
Authors	:	Onesti, S.; Brick, P.
Deposited on	:	1995-05-03
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

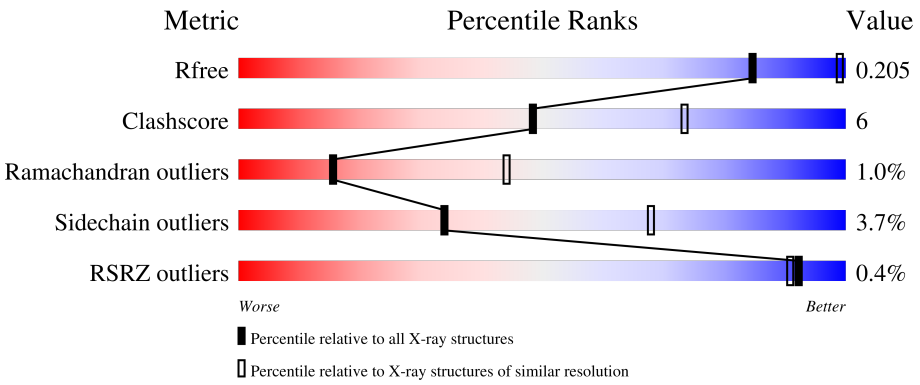
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	504	81% 13% • •
1	B	504	80% 15% • •
1	C	504	% 79% 15% • •

2 Entry composition (i)

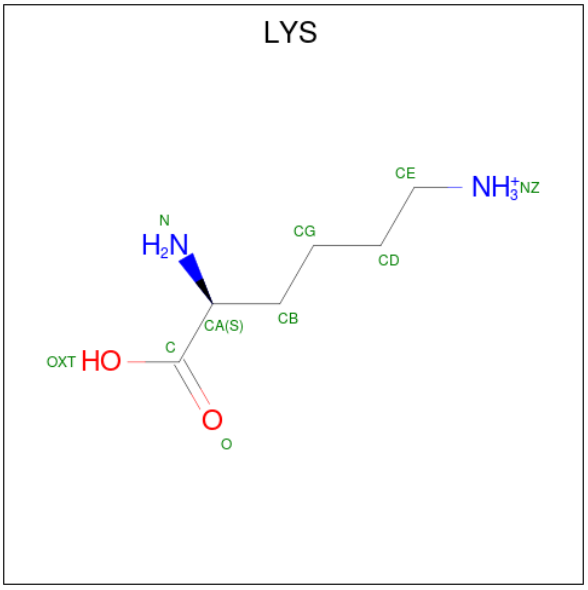
There are 3 unique types of molecules in this entry. The entry contains 11751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LYSYL-TRNA SYNTHETASE (LYSU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	3785	2404	656	707	18	0	0	0
1	B	483	3781	2400	654	709	18	0	0	0
1	C	482	3783	2402	656	707	18	0	0	0

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	6	2	1	0	0
2	B	1	9	6	2	1	0	0
2	C	1	9	6	2	1	0	0

- Molecule 3 is water.

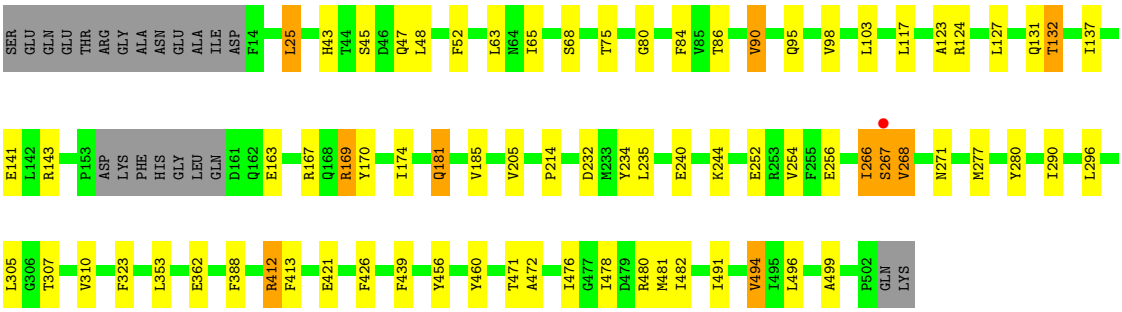
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	128	128	128	0	0
			Total	O		
3	B	124	124	124	0	0
			Total	O		
3	C	123	123	123	0	0

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.

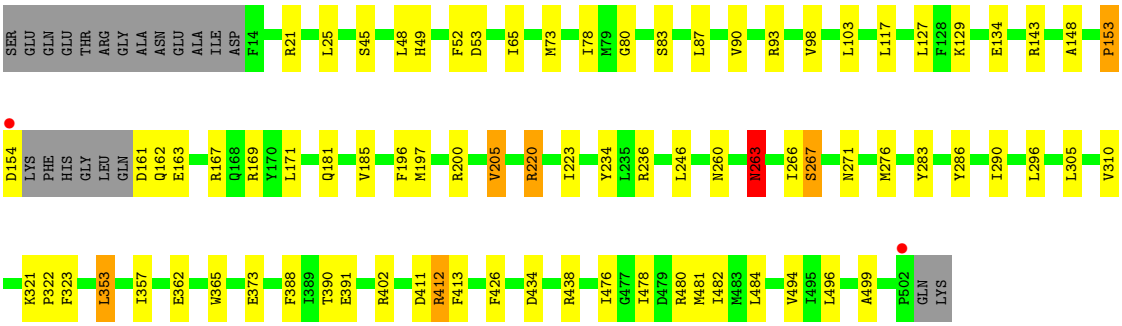
• Molecule 1: LYSYL-TRNA SYNTHETASE (LYSU)

Chain A:



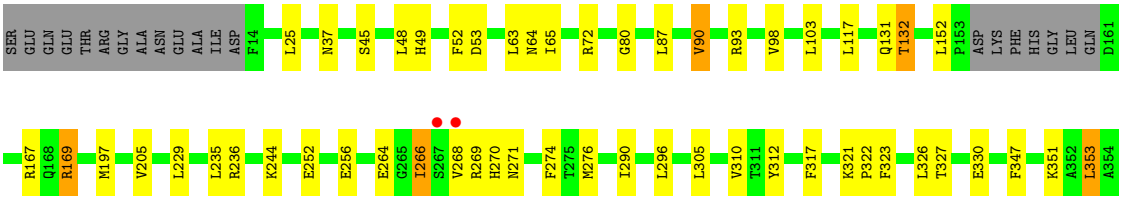
• Molecule 1: LYSYL-TRNA SYNTHETASE (LYSU)

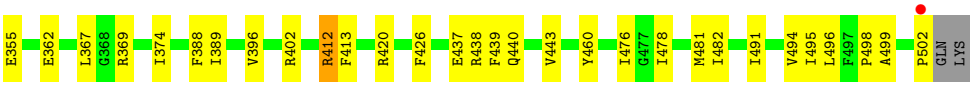
Chain B:



• Molecule 1: LYSYL-TRNA SYNTHETASE (LYSU)

Chain C:




E355
E362
L367
G368
R369
I374
F388
I389
V396
R402
R412
F413
R420
F426
E437
R438
F439
Q440
V443
Y460
I476
G477
I478
M481
I482
I491
V494
I495
L496
F497
P498
A499
P502
GLN
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	144.27Å 257.80Å 182.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.80 11.98 – 2.82	Depositor EDS
% Data completeness (in resolution range)	92.8 (12.00-2.80) 94.4 (11.98-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 2.83Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.193 , 0.238 0.168 , 0.205	Depositor DCC
R_{free} test set	3103 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.056 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11751	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0/3861	0.61	0/5227
1	B	0.38	0/3856	0.60	0/5222
1	C	0.39	0/3859	0.62	1/5224 (0.0%)
All	All	0.39	0/11576	0.61	1/15673 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	264	GLU	N-CA-C	-5.36	96.53	111.00

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	3785	0	3653	42	0
1	B	3781	0	3631	49	0
1	C	3783	0	3646	51	0
2	A	9	0	12	0	0
2	B	9	0	12	1	0
2	C	9	0	12	0	0
3	A	128	0	0	1	0
3	B	124	0	0	3	0
3	C	123	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11751	0	10966	135	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 6.

All (135) 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:169:ARG:HG3	1:A:496:LEU:O	1.76	0.85
1:C:169:ARG:HG3	1:C:496:LEU:O	1.85	0.77
1:B:200:ARG:HG2	1:B:200:ARG:HH11	1.51	0.74
1:C:131:GLN:O	1:C:132:THR:HG23	1.89	0.72
1:A:131:GLN:O	1:A:132:THR:HG23	1.90	0.72
1:C:402:ARG:HG3	1:C:438:ARG:NH2	2.05	0.71
1:C:369:ARG:HD3	3:C:587:HOH:O	1.94	0.68
1:A:25:LEU:HB3	3:A:607:HOH:O	1.94	0.67
1:C:37:ASN:HB2	3:C:599:HOH:O	1.95	0.67
1:B:390:THR:HG22	1:B:391:GLU:HG3	1.78	0.66
1:B:412:ARG:HG2	1:B:426:PHE:HB3	1.79	0.65
1:A:163:GLU:O	1:A:167:ARG:HG3	1.97	0.64
1:C:321:LYS:HG3	1:C:322:PRO:HD2	1.78	0.64
1:A:271:ASN:HD21	1:A:499:ALA:H	1.45	0.64
1:B:271:ASN:HD21	1:B:499:ALA:H	1.47	0.63
1:B:260:ASN:ND2	1:B:276:MET:HG3	2.13	0.62
1:A:476:ILE:HG21	1:A:481:MET:HE3	1.82	0.62
1:B:305:LEU:HD12	1:B:310:VAL:HG22	1.82	0.61
1:C:482:ILE:HB	1:C:494:VAL:HG21	1.82	0.61
1:C:52:PHE:CE1	1:C:65:ILE:HD13	2.35	0.61
1:B:52:PHE:CE1	1:B:65:ILE:HD13	2.36	0.61
1:B:476:ILE:HG21	1:B:481:MET:HE3	1.82	0.60
1:B:163:GLU:O	1:B:167:ARG:HG3	2.02	0.60
1:B:153:PRO:HG3	1:B:171:LEU:HD22	1.83	0.60
1:C:271:ASN:HD21	1:C:499:ALA:H	1.49	0.59
1:C:412:ARG:HG2	1:C:426:PHE:HB3	1.85	0.59
1:A:266:ILE:HG13	1:C:229:LEU:HD21	1.84	0.58
1:A:421:GLU:O	1:A:480:ARG:NH1	2.36	0.58
1:C:412:ARG:HA	1:C:426:PHE:HB3	1.86	0.56
1:B:402:ARG:HG3	1:B:438:ARG:NH2	2.20	0.56
1:C:197:MET:HA	1:C:197:MET:HE2	1.88	0.55
1:C:351:LYS:O	1:C:355:GLU:HG3	2.07	0.55
1:B:412:ARG:HA	1:B:426:PHE:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:ILE:O	1:C:482:ILE:HG12	2.06	0.54
1:A:52:PHE:CE1	1:A:65:ILE:HD13	2.42	0.54
1:C:396:VAL:HG12	3:C:587:HOH:O	2.07	0.54
1:C:63:LEU:O	1:C:65:ILE:N	2.41	0.54
1:C:323:PHE:CD1	1:C:323:PHE:N	2.76	0.54
1:B:49:HIS:HE1	1:B:93:ARG:O	1.91	0.53
1:A:412:ARG:HA	1:A:426:PHE:HB3	1.90	0.53
1:B:200:ARG:HG2	1:B:200:ARG:NH1	2.22	0.52
1:B:365:TRP:CZ3	1:B:373:GLU:HG3	2.45	0.52
1:A:478:ILE:O	1:A:482:ILE:HG12	2.10	0.52
1:B:484:LEU:HD21	3:B:555:HOH:O	2.09	0.51
1:B:49:HIS:O	1:B:53:ASP:HB2	2.11	0.51
1:A:181:GLN:O	1:A:185:VAL:HG23	2.11	0.50
1:B:78:ILE:HA	1:B:83:SER:OG	2.12	0.50
1:A:235:LEU:HD21	1:C:235:LEU:HD11	1.93	0.50
1:C:98:VAL:HG13	1:C:103:LEU:HD11	1.93	0.50
1:B:478:ILE:O	1:B:482:ILE:HG12	2.12	0.50
1:C:269:ARG:HA	1:C:491:ILE:HG22	1.94	0.50
1:A:45:SER:HA	1:A:48:LEU:HD12	1.94	0.49
1:A:98:VAL:HG13	1:A:103:LEU:HD11	1.94	0.49
1:B:205:VAL:HG11	1:B:246:LEU:CD1	2.42	0.49
1:C:49:HIS:HE1	3:C:604:HOH:O	1.94	0.49
1:C:244:LYS:HD2	1:C:460:TYR:OH	2.13	0.49
1:A:75:THR:OG1	1:A:86:THR:HB	2.13	0.49
1:A:84:PHE:HB3	1:A:95:GLN:HE21	1.76	0.49
1:B:426:PHE:CZ	2:B:505:LYS:HE2	2.48	0.48
1:A:170:TYR:O	1:A:174:ILE:HG13	2.13	0.48
1:B:480:ARG:HG3	1:B:480:ARG:HH11	1.78	0.48
1:B:276:MET:HE2	3:B:542:HOH:O	2.13	0.48
1:C:305:LEU:HD12	1:C:310:VAL:HG22	1.94	0.48
1:A:214:PRO:HD3	1:A:234:TYR:CD1	2.49	0.48
1:A:323:PHE:CD1	1:A:323:PHE:N	2.82	0.48
1:C:49:HIS:O	1:C:53:ASP:HB2	2.14	0.48
1:C:353:LEU:HD13	1:C:374:ILE:HD13	1.96	0.47
1:A:266:ILE:HD11	1:C:229:LEU:HD11	1.94	0.47
1:A:290:ILE:HG23	1:A:388:PHE:CE2	2.49	0.47
1:C:266:ILE:CB	1:C:270:HIS:HB3	2.44	0.47
1:C:87:LEU:O	1:C:93:ARG:HA	2.15	0.47
1:B:413:PHE:C	1:B:413:PHE:CD1	2.88	0.47
1:B:390:THR:CG2	1:B:391:GLU:HG3	2.45	0.47
1:A:413:PHE:CD1	1:A:413:PHE:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:PHE:HA	1:C:367:LEU:HD13	1.97	0.46
1:C:495:ILE:O	1:C:498:PRO:HD3	2.15	0.46
1:A:244:LYS:HD2	1:A:460:TYR:OH	2.16	0.46
1:C:491:ILE:O	1:C:494:VAL:HG12	2.16	0.46
1:B:45:SER:HA	1:B:48:LEU:HD12	1.97	0.45
1:C:327:THR:OG1	1:C:330:GLU:HG3	2.16	0.45
1:B:220:ARG:HB3	1:B:263:ASN:HB3	1.98	0.45
1:B:353:LEU:O	1:B:357:ILE:HG13	2.17	0.45
1:C:413:PHE:C	1:C:413:PHE:CD1	2.90	0.45
1:B:480:ARG:HG3	1:B:480:ARG:NH1	2.32	0.45
1:A:252:GLU:H	1:C:90:VAL:HG13	1.81	0.44
1:B:87:LEU:O	1:B:93:ARG:HA	2.17	0.44
1:B:290:ILE:HG23	1:B:388:PHE:CE2	2.51	0.44
1:B:223:ILE:HG12	1:B:234:TYR:CE2	2.52	0.44
1:A:471:THR:HG22	1:A:472:ALA:N	2.32	0.44
1:B:196:PHE:CE1	1:B:197:MET:HE1	2.53	0.44
1:B:266:ILE:O	1:B:267:SER:CB	2.65	0.44
1:B:323:PHE:CD1	1:B:323:PHE:N	2.84	0.44
1:B:161:ASP:O	1:B:163:GLU:N	2.52	0.43
1:C:323:PHE:N	1:C:323:PHE:HD1	2.17	0.43
1:C:72:ARG:HD3	1:C:152:LEU:HD21	2.01	0.43
1:C:312:TYR:HB3	1:C:317:PHE:CE2	2.53	0.43
1:C:437:GLU:O	1:C:440:GLN:HB2	2.18	0.43
1:B:286:TYR:CD1	1:B:411:ASP:HB3	2.54	0.43
1:A:266:ILE:CD1	1:C:229:LEU:HD11	2.48	0.43
1:B:21:ARG:HH12	1:B:148:ALA:HB3	1.83	0.43
1:A:43:HIS:HA	1:A:47:GLN:OE1	2.19	0.42
1:A:256:GLU:O	1:A:277:MET:HA	2.19	0.42
1:B:98:VAL:HG13	1:B:103:LEU:HD11	2.00	0.42
1:A:240:GLU:HG3	1:A:280:TYR:OH	2.19	0.42
1:A:412:ARG:HG3	1:A:426:PHE:CD2	2.54	0.42
1:C:45:SER:HA	1:C:48:LEU:HD12	2.02	0.42
1:A:90:VAL:HG13	1:C:252:GLU:HB2	2.02	0.42
1:B:129:LYS:HA	1:B:134:GLU:O	2.20	0.42
1:B:283:TYR:HA	3:B:543:HOH:O	2.19	0.42
1:B:390:THR:CG2	1:B:391:GLU:N	2.83	0.42
1:A:48:LEU:HD22	1:A:127:LEU:HD21	2.02	0.42
1:B:181:GLN:O	1:B:185:VAL:HG23	2.19	0.42
1:C:274:PHE:CE2	1:C:276:MET:HG2	2.55	0.42
1:C:256:GLU:HG3	3:C:538:HOH:O	2.19	0.41
1:A:476:ILE:CG2	1:A:481:MET:HE3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HB3	1:A:141:GLU:HB3	2.03	0.41
1:A:439:PHE:HB3	1:A:456:TYR:CD2	2.56	0.41
1:B:73:MET:O	1:B:117:LEU:O	2.37	0.41
1:A:267:SER:O	1:A:268:VAL:CB	2.69	0.41
1:B:48:LEU:HD22	1:B:127:LEU:HD21	2.03	0.41
1:C:235:LEU:HD23	1:C:235:LEU:HA	1.87	0.41
1:A:90:VAL:CG1	1:C:252:GLU:H	2.33	0.41
1:A:68:SER:HA	1:A:123:ALA:O	2.21	0.41
1:B:169:ARG:NE	1:B:496:LEU:O	2.51	0.41
1:B:434:ASP:O	1:B:438:ARG:HG3	2.21	0.41
1:A:305:LEU:HD12	1:A:310:VAL:HG22	2.03	0.41
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.86	0.40
1:A:127:LEU:HD23	1:A:137:ILE:HG12	2.02	0.40
1:B:321:LYS:HG3	1:B:322:PRO:HD2	2.03	0.40
1:C:412:ARG:CG	1:C:426:PHE:HB3	2.50	0.40
1:C:326:LEU:O	1:C:389:ILE:HA	2.21	0.40
1:C:439:PHE:O	1:C:443:VAL:HG23	2.22	0.40
1:C:476:ILE:HG21	1:C:481:MET:HE1	2.03	0.40
1:A:491:ILE:O	1:A:494:VAL:HG12	2.22	0.40
1:C:290:ILE:HG23	1:C:388:PHE:CE2	2.56	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	478/504 (95%)	461 (96%)	13 (3%)	4 (1%)	19	49
1	B	479/504 (95%)	457 (95%)	17 (4%)	5 (1%)	15	44
1	C	478/504 (95%)	457 (96%)	16 (3%)	5 (1%)	15	44
All	All	1435/1512 (95%)	1375 (96%)	46 (3%)	14 (1%)	15	44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	THR
1	A	267	SER
1	A	268	VAL
1	B	162	GLN
1	B	267	SER
1	C	132	THR
1	A	80	GLY
1	B	80	GLY
1	B	263	ASN
1	C	64	ASN
1	C	80	GLY
1	C	266	ILE
1	B	153	PRO
1	C	268	VAL

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	387/430 (90%)	370 (96%)	17 (4%)	28	61
1	B	384/430 (89%)	371 (97%)	13 (3%)	37	71
1	C	386/430 (90%)	373 (97%)	13 (3%)	37	71
All	All	1157/1290 (90%)	1114 (96%)	43 (4%)	34	68

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	63	LEU
1	A	90	VAL
1	A	117	LEU
1	A	143	ARG
1	A	169	ARG
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	232	ASP
1	A	254	VAL
1	A	266	ILE
1	A	296	LEU
1	A	307	THR
1	A	353	LEU
1	A	362	GLU
1	A	412	ARG
1	A	494	VAL
1	B	25	LEU
1	B	90	VAL
1	B	143	ARG
1	B	154	ASP
1	B	205	VAL
1	B	220	ARG
1	B	236	ARG
1	B	263	ASN
1	B	296	LEU
1	B	353	LEU
1	B	362	GLU
1	B	412	ARG
1	B	494	VAL
1	C	25	LEU
1	C	90	VAL
1	C	117	LEU
1	C	167	ARG
1	C	169	ARG
1	C	205	VAL
1	C	236	ARG
1	C	296	LEU
1	C	353	LEU
1	C	362	GLU
1	C	412	ARG
1	C	420	ARG
1	C	502	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	211	GLN

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Mol	Chain	Res	Type
1	A	271	ASN
1	B	49	HIS
1	B	211	GLN
1	B	263	ASN
1	B	271	ASN
1	C	211	GLN
1	C	271	ASN
1	C	382	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands 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	$\#\|Z\| > 2$
2	LYS	A	505	-	7,8,9	0.44	0	3,8,10	0.59	0
2	LYS	C	505	-	7,8,9	0.41	0	3,8,10	0.61	0
2	LYS	B	505	-	7,8,9	0.55	0	3,8,10	0.37	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
2	LYS	A	505	-	-	1/6/7/9	-
2	LYS	C	505	-	-	1/6/7/9	-
2	LYS	B	505	-	-	1/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	505	LYS	CA-CB-CG-CD
2	C	505	LYS	CG-CD-CE-NZ
2	A	505	LYS	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	LYS	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	482/504 (95%)	-1.09	1 (0%)	95	94	4, 20, 62, 88	0
1	B	483/504 (95%)	-1.04	2 (0%)	92	91	4, 21, 68, 93	0
1	C	482/504 (95%)	-1.03	3 (0%)	89	86	3, 21, 67, 99	0
All	All	1447/1512 (95%)	-1.06	6 (0%)	92	91	3, 21, 67, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	VAL	4.8
1	C	502	PRO	3.4
1	B	502	PRO	2.8
1	B	154	ASP	2.6
1	A	267	SER	2.5
1	C	267	SER	2.2

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 monosaccharides 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(Å^2)	Q<0.9
2	LYS	A	505	9/10	0.95	0.14	8,12,15,19	0
2	LYS	B	505	9/10	0.95	0.19	13,14,21,26	0
2	LYS	C	505	9/10	0.96	0.17	10,16,21,23	0

6.5 Other polymers (i)

There are no such residues in this entry.