Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 02:40 AM JST

PDB ID	:	5YYN
Title	:	Crystal structures of E.coli arginyl-trna synthetase (argrs) in complex with substrate TRNA(Arg)
Authors	:	Zhou, M.; Ye, S.; Stephen, P.; Zhang, R.G.; Wang, E.D.; Giege, R.; Lin, S.X.
Deposited on	:	2017-12-10
Resolution	:	3.00 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 (1)) were used in the production of this report:

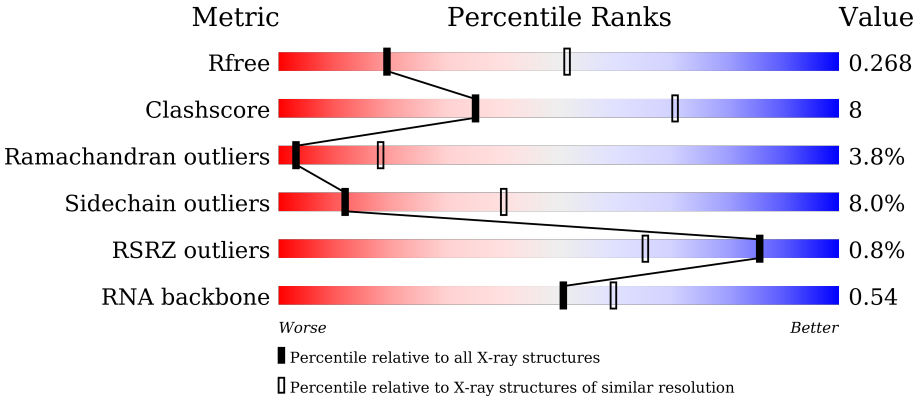
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

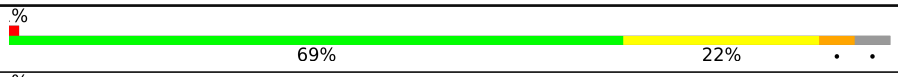
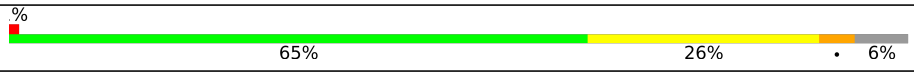
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=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	586	
1	C	586	
2	B	77	
2	D	77	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11523 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 Arginine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	4442	2811	768	838	25	0	0	0
1	C	553	4331	2742	748	815	26	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP P11875
A	-7	HIS	-	expression tag	UNP P11875
A	-6	HIS	-	expression tag	UNP P11875
A	-5	HIS	-	expression tag	UNP P11875
A	-4	HIS	-	expression tag	UNP P11875
A	-3	HIS	-	expression tag	UNP P11875
A	-2	GLY	-	expression tag	UNP P11875
A	-1	GLY	-	expression tag	UNP P11875
A	0	ALA	-	expression tag	UNP P11875
C	-8	HIS	-	expression tag	UNP P11875
C	-7	HIS	-	expression tag	UNP P11875
C	-6	HIS	-	expression tag	UNP P11875
C	-5	HIS	-	expression tag	UNP P11875
C	-4	HIS	-	expression tag	UNP P11875
C	-3	HIS	-	expression tag	UNP P11875
C	-2	GLY	-	expression tag	UNP P11875
C	-1	GLY	-	expression tag	UNP P11875
C	0	ALA	-	expression tag	UNP P11875

- Molecule 2 is a RNA chain called TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	63	1349	601	243	442	63	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	64	1369	610	245	450	64	0	0	0

- Molecule 3 is water.

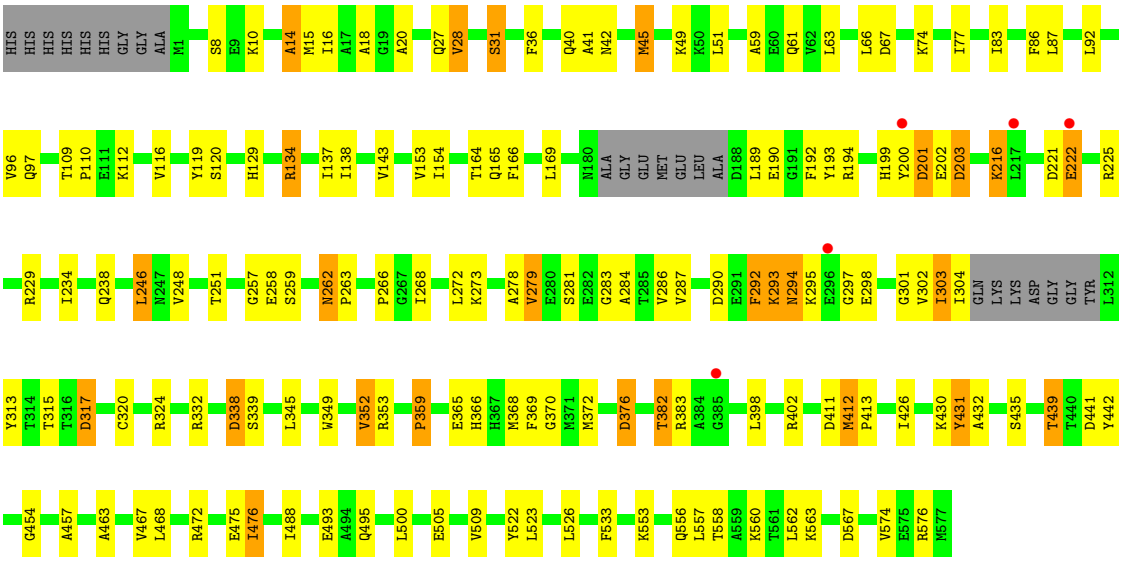
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	10	10	10	0	0
			Total	O		
3	B	4	4	4	0	0
			Total	O		
3	C	10	10	10	0	0
			Total	O		
3	D	8	8	8	0	0

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.

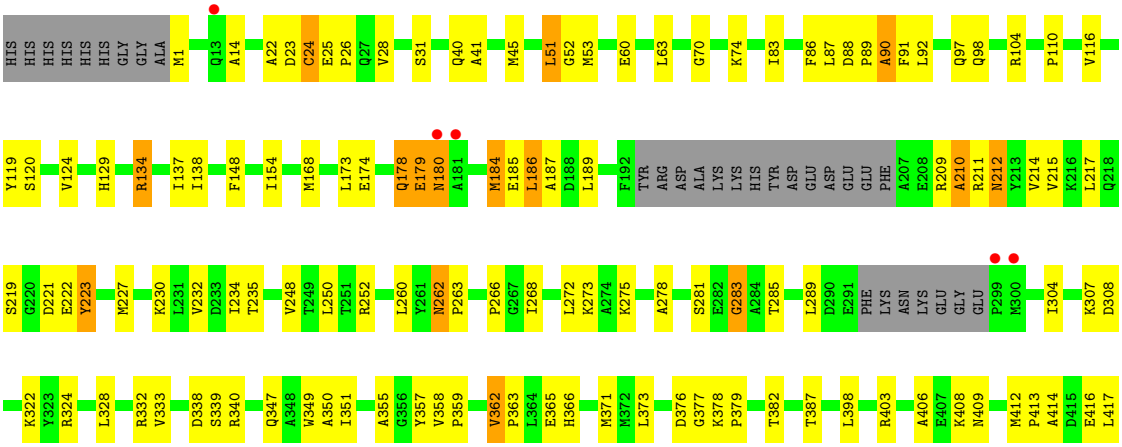
• Molecule 1: Arginine–tRNA ligase

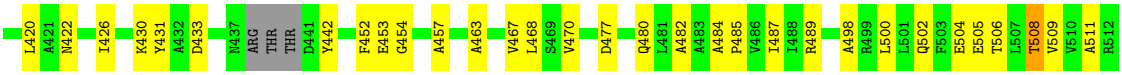
Chain A:



• Molecule 1: Arginine–tRNA ligase

Chain C:



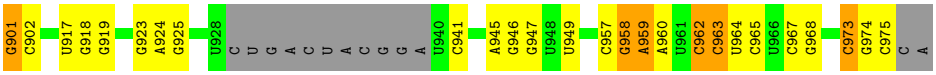


- Molecule 2: TRNA

Chain B:

- Molecule 2: TRNA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	102.24Å 102.24Å 480.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.15 – 3.00 33.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (33.15-3.00) 89.3 (33.15-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.220 , 0.268 0.220 , 0.268	Depositor DCC
R_{free} test set	2728 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11523	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.23	0/4523	0.44	0/6113
1	C	0.23	0/4407	0.43	0/5955
2	B	0.33	1/1507 (0.1%)	0.72	0/2344
2	D	0.33	1/1529 (0.1%)	0.73	0/2378
All	All	0.26	2/11966 (0.0%)	0.53	0/16790

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	G	OP3-P	-10.73	1.48	1.61
2	D	901	G	OP3-P	-10.66	1.48	1.61

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	4442	0	4420	84	0
1	C	4331	0	4327	83	0
2	B	1349	0	681	4	0
2	D	1369	0	691	8	0
3	A	10	0	0	1	0
3	B	4	0	0	0	0
3	C	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	8	0	0	0	0
All	All	11523	0	10119	175	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 8.

All (175) 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)
2:D:901:G:O6	2:D:973:C:N4	2.16	0.78
1:C:41:ALA:HB3	1:C:83:ILE:HB	1.68	0.76
1:A:317:ASP:OD1	1:A:317:ASP:N	2.18	0.76
1:A:14:ALA:O	1:A:16:ILE:N	2.19	0.76
1:C:137:ILE:HD13	1:C:430:LYS:HA	1.70	0.74
1:A:41:ALA:HB3	1:A:83:ILE:HB	1.71	0.73
1:A:137:ILE:HD13	1:A:430:LYS:HA	1.71	0.72
1:A:370:GLY:HA3	1:A:441:ASP:H	1.54	0.70
1:C:124:VAL:HA	1:C:235:THR:HG21	1.77	0.67
1:C:541:SER:N	3:C:601:HOH:O	2.11	0.65
1:A:166:PHE:HA	1:A:169:LEU:HB2	1.79	0.64
1:A:294:ASN:N	1:A:294:ASN:OD1	2.31	0.63
1:C:484:ALA:O	1:C:553:LYS:NZ	2.29	0.63
1:A:411:ASP:OD1	1:C:252:ARG:NH1	2.31	0.62
1:A:27:GLN:HB2	1:A:42:ASN:HB2	1.80	0.62
1:C:409:ASN:ND2	1:C:412:MET:SD	2.73	0.62
1:A:134:ARG:HH11	1:A:138:ILE:HD11	1.66	0.61
1:C:116:VAL:HG11	1:C:324:ARG:HD2	1.82	0.60
1:A:74:LYS:HB3	1:A:86:PHE:HB2	1.84	0.59
1:A:273:LYS:HG2	1:A:278:ALA:HB3	1.83	0.59
1:A:190:GLU:O	1:A:194:ARG:NH1	2.32	0.59
1:A:203:ASP:OD1	1:A:203:ASP:N	2.36	0.59
1:A:116:VAL:HG22	1:A:154:ILE:HB	1.85	0.59
1:A:262:ASN:H	1:A:263:PRO:HD2	1.67	0.58
1:A:292:PHE:HD1	1:A:293:LYS:HG2	1.68	0.58
1:C:340:ARG:NH1	1:C:371:MET:SD	2.75	0.58
1:A:369:PHE:HA	1:A:439:THR:HA	1.85	0.58
1:C:281:SER:O	1:C:283:GLY:N	2.34	0.57
1:C:338:ASP:OD1	1:C:339:SER:N	2.38	0.57
1:A:222:GLU:HA	1:A:225:ARG:HB3	1.86	0.57
1:C:87:LEU:HD13	1:C:92:LEU:HD21	1.87	0.57
1:C:262:ASN:H	1:C:263:PRO:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HB3	1:A:248:VAL:HG23	1.87	0.56
1:C:210:ALA:O	1:C:212:ASN:N	2.39	0.55
1:C:74:LYS:HB3	1:C:86:PHE:HB2	1.88	0.55
1:A:303:ILE:HG23	1:A:304:ILE:HG13	1.89	0.55
1:A:116:VAL:HG11	1:A:324:ARG:HD2	1.88	0.55
1:C:504:GLU:O	1:C:508:THR:OG1	2.25	0.54
1:A:500:LEU:HD13	1:A:557:LEU:HD23	1.90	0.54
1:A:563:LYS:NZ	1:A:567:ASP:OD1	2.40	0.54
1:C:212:ASN:N	1:C:212:ASN:OD1	2.29	0.54
1:C:134:ARG:NH1	1:C:433:ASP:O	2.41	0.54
1:C:332:ARG:NH2	1:C:511:ALA:O	2.35	0.54
1:C:378:LYS:HD2	1:C:379:PRO:HD2	1.90	0.54
1:A:59:ALA:HB1	1:A:77:ILE:HD12	1.90	0.53
1:A:431:TYR:HB3	1:A:457:ALA:HB2	1.90	0.53
1:C:116:VAL:HG22	1:C:154:ILE:HB	1.90	0.53
1:A:574:VAL:HG12	1:A:576:ARG:H	1.73	0.53
1:C:538:PRO:O	1:C:551:ARG:NH1	2.40	0.53
1:A:439:THR:O	1:A:439:THR:OG1	2.24	0.53
1:C:60:GLU:HA	1:C:63:LEU:HG	1.89	0.53
1:C:482:ALA:O	1:C:553:LYS:NZ	2.42	0.52
1:A:338:ASP:OD1	1:A:339:SER:N	2.44	0.51
1:A:45:MET:SD	1:A:45:MET:N	2.79	0.51
1:A:238:GLN:OE1	1:C:403:ARG:NH1	2.44	0.51
1:C:454:GLY:HA2	2:D:925:G:H4'	1.93	0.50
1:A:412:MET:HG3	1:A:413:PRO:HD2	1.92	0.50
1:C:431:TYR:HB3	1:C:457:ALA:HB2	1.93	0.50
1:C:500:LEU:HD21	1:C:558:THR:HB	1.92	0.50
1:A:292:PHE:HE1	1:A:297:GLY:H	1.60	0.49
1:C:324:ARG:HD3	1:C:328:LEU:HD12	1.93	0.49
1:A:366:HIS:CE1	1:A:368:MET:HB3	2.46	0.49
1:C:51:LEU:HD12	1:C:53:MET:HG2	1.94	0.49
1:C:406:ALA:HB2	1:C:417:LEU:HD11	1.94	0.49
1:A:320:CYS:O	1:A:324:ARG:HG2	2.13	0.49
1:A:382:THR:OG1	1:A:383:ARG:N	2.46	0.49
1:C:124:VAL:HG11	1:C:232:VAL:HG22	1.94	0.49
1:C:88:ASP:O	1:C:90:ALA:N	2.43	0.49
1:A:8:SER:HA	1:A:28:VAL:HG21	1.94	0.48
1:A:268:ILE:O	1:A:272:LEU:HB2	2.13	0.48
1:C:31:SER:HA	1:C:40:GLN:HG3	1.95	0.48
1:C:347:GLN:O	1:C:351:ILE:HG13	2.12	0.48
1:A:202:GLU:HA	1:A:203:ASP:HA	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:VAL:HG12	1:C:250:LEU:H	1.79	0.48
1:A:97:GLN:OE1	1:A:553:LYS:NZ	2.31	0.47
1:A:293:LYS:HE3	1:A:295:LYS:HB3	1.96	0.47
1:C:116:VAL:HB	1:C:333:VAL:HG13	1.96	0.47
1:A:134:ARG:HG3	1:A:442:TYR:CZ	2.49	0.47
1:A:28:VAL:HA	1:A:40:GLN:O	2.14	0.47
1:A:488:ILE:HG23	1:A:493:GLU:HB2	1.95	0.47
1:A:523:LEU:HD22	1:A:562:LEU:HD23	1.96	0.47
1:A:353:ARG:NH1	1:A:359:PRO:O	2.48	0.47
1:C:104:ARG:NH2	1:C:148:PHE:O	2.43	0.47
1:C:273:LYS:HD2	1:C:278:ALA:HB3	1.96	0.47
1:A:345:LEU:HD12	1:A:366:HIS:CD2	2.50	0.47
1:C:477:ASP:OD1	1:C:477:ASP:N	2.42	0.47
2:D:962:C:H2'	2:D:963:C:H6	1.81	0.46
1:C:134:ARG:HH11	1:C:138:ILE:HD11	1.79	0.46
1:C:178:GLN:H	1:C:178:GLN:HG3	1.54	0.46
1:C:184:MET:SD	1:C:184:MET:N	2.89	0.46
1:A:63:LEU:HA	1:A:66:LEU:HB3	1.98	0.45
1:A:290:ASP:N	1:A:290:ASP:OD1	2.49	0.45
1:C:22:ALA:O	1:C:24:CYS:N	2.49	0.45
1:A:216:LYS:H	1:A:216:LYS:HG2	1.54	0.45
1:A:143:VAL:HG13	1:A:153:VAL:HG11	1.99	0.45
1:C:545:GLU:HG3	1:C:549:ASN:HD21	1.81	0.45
1:C:179:GLU:HB3	1:C:180:ASN:H	1.61	0.45
1:C:422:ASN:O	1:C:426:ILE:HG12	2.16	0.45
1:A:454:GLY:HA2	2:B:925:G:H4'	1.97	0.45
1:C:408:LYS:HE3	1:C:452:PHE:CE1	2.52	0.45
2:D:962:C:H2'	2:D:963:C:C6	2.51	0.45
1:C:543:GLU:CD	1:C:543:GLU:H	2.21	0.45
1:A:372:MET:HG2	1:A:442:TYR:CE2	2.52	0.45
1:C:70:GLY:O	1:C:91:PHE:HB2	2.17	0.45
1:C:285:THR:O	1:C:304:ILE:HG12	2.18	0.44
1:C:463:ALA:O	1:C:467:VAL:HG23	2.18	0.44
2:D:958:G:HO2'	2:D:959:A:P	2.40	0.44
1:A:129:HIS:HB3	3:A:605:HOH:O	2.18	0.44
1:A:332:ARG:NE	1:A:365:GLU:OE2	2.48	0.44
1:A:257:GLY:O	1:A:259:SER:N	2.46	0.44
1:A:287:VAL:N	1:A:298:GLU:OE2	2.51	0.44
2:B:910:G:H1	2:B:926:C:H42	1.64	0.44
1:C:467:VAL:HG22	1:C:530:PHE:CE2	2.52	0.44
1:C:484:ALA:HA	1:C:485:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:ALA:O	1:C:502:GLN:HG3	2.17	0.44
1:A:292:PHE:HD1	1:A:293:LYS:H	1.66	0.44
1:A:430:LYS:O	1:A:432:ALA:N	2.49	0.44
1:C:398:LEU:HD21	1:C:422:ASN:HA	1.98	0.43
1:C:416:GLU:HG2	1:C:420:LEU:HD13	2.00	0.43
1:A:398:LEU:O	1:A:402:ARG:HG3	2.18	0.43
1:C:513:GLU:HB3	1:C:515:THR:HG23	2.00	0.43
1:A:293:LYS:HG3	1:A:295:LYS:H	1.84	0.43
1:A:87:LEU:HD13	1:A:92:LEU:HD21	2.01	0.43
1:A:281:SER:C	1:A:283:GLY:H	2.21	0.43
2:B:958:G:O2'	2:B:959:A:OP1	2.34	0.43
1:C:268:ILE:HD13	1:C:268:ILE:HA	1.91	0.43
2:D:945:A:H2'	2:D:946:G:O4'	2.19	0.43
2:D:967:C:H2'	2:D:968:G:C8	2.53	0.43
1:C:506:THR:HG21	1:C:522:TYR:CG	2.54	0.43
1:A:165:GLN:HG3	1:A:193:TYR:HE1	1.84	0.42
1:C:322:LYS:HZ2	1:C:357:TYR:HD1	1.67	0.42
1:A:16:ILE:HA	1:A:20:ALA:HB3	2.01	0.42
2:B:962:C:H2'	2:B:963:C:H6	1.83	0.42
1:A:221:ASP:N	1:A:221:ASP:OD1	2.51	0.42
1:A:556:GLN:O	1:A:560:LYS:HG3	2.19	0.42
1:C:186:LEU:HB3	1:C:187:ALA:H	1.46	0.42
1:C:376:ASP:N	1:C:376:ASP:OD1	2.52	0.42
1:A:286:VAL:HB	1:A:298:GLU:OE2	2.20	0.42
1:A:317:ASP:HA	1:A:320:CYS:HB3	2.00	0.42
1:C:148:PHE:CZ	1:C:564:LEU:HD21	2.54	0.42
1:A:493:GLU:HG2	1:A:533:PHE:HE1	1.84	0.42
1:C:349:TRP:CZ3	1:C:366:HIS:HB2	2.54	0.42
1:A:279:VAL:O	1:A:286:VAL:HG22	2.19	0.41
1:C:51:LEU:O	1:C:53:MET:N	2.46	0.41
1:A:284:ALA:HB2	1:A:303:ILE:HD13	2.01	0.41
1:C:230:LYS:HE3	1:C:230:LYS:HB2	1.88	0.41
1:C:97:GLN:HE22	1:C:553:LYS:NZ	2.18	0.41
1:C:217:LEU:HA	1:C:221:ASP:HB2	2.01	0.41
1:C:173:LEU:HD21	1:C:230:LYS:HD3	2.02	0.41
1:C:212:ASN:O	1:C:215:VAL:HG22	2.21	0.41
1:A:31:SER:HB3	1:A:36:PHE:HB2	2.03	0.41
1:C:275:LYS:NZ	1:C:355:ALA:O	2.48	0.41
1:C:373:LEU:HD13	1:C:377:GLY:HA2	2.03	0.41
1:C:134:ARG:HG3	1:C:442:TYR:CZ	2.56	0.41
1:C:174:GLU:OE2	1:C:223:TYR:OH	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:ILE:HD13	1:C:489:ARG:NH1	2.36	0.41
1:A:109:THR:HA	1:A:110:PRO:HD3	1.90	0.41
1:A:281:SER:O	1:A:283:GLY:N	2.48	0.41
1:C:25:GLU:HA	1:C:26:PRO:HD2	1.97	0.41
1:C:362:VAL:HA	1:C:363:PRO:HD3	1.87	0.41
1:A:463:ALA:O	1:A:467:VAL:HG23	2.21	0.41
1:A:505:GLU:O	1:A:509:VAL:HG23	2.21	0.41
1:A:522:TYR:O	1:A:526:LEU:N	2.52	0.41
1:C:283:GLY:O	1:C:307:LYS:HA	2.21	0.41
1:C:289:LEU:HD13	1:C:350:ALA:HB3	2.03	0.41
1:A:18:ALA:HB1	1:A:61:GLN:HG2	2.03	0.40
1:A:189:LEU:HD23	1:A:234:ILE:HG22	2.02	0.40
1:A:292:PHE:CD1	1:A:293:LYS:HG2	2.53	0.40
1:A:349:TRP:HA	1:A:352:VAL:HG23	2.02	0.40
1:C:505:GLU:O	1:C:509:VAL:HG23	2.21	0.40
1:C:332:ARG:NE	1:C:365:GLU:OE2	2.54	0.40
2:D:964:U:H2'	2:D:965:C:C6	2.57	0.40
1:A:10:LYS:NZ	1:A:67:ASP:O	2.34	0.40
1:A:199:HIS:O	1:A:201:ASP:N	2.44	0.40
1:C:60:GLU:OE1	1:C:60:GLU:N	2.45	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	557/586 (95%)	463 (83%)	74 (13%)	20 (4%)	3 19
1	C	545/586 (93%)	461 (85%)	62 (11%)	22 (4%)	3 17
All	All	1102/1172 (94%)	924 (84%)	136 (12%)	42 (4%)	3 18

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	476	ILE
1	C	211	ARG
1	C	413	PRO
1	A	14	ALA
1	A	201	ASP
1	A	303	ILE
1	A	435	SER
1	C	219	SER
1	C	262	ASN
1	C	536	HIS
1	A	120	SER
1	A	200	TYR
1	A	222	GLU
1	A	258	GLU
1	A	262	ASN
1	A	266	PRO
1	A	359	PRO
1	A	376	ASP
1	A	431	TYR
1	C	23	ASP
1	C	90	ALA
1	C	120	SER
1	C	186	LEU
1	C	359	PRO
1	C	540	LEU
1	C	541	SER
1	A	49	LYS
1	A	112	LYS
1	A	472	ARG
1	C	283	GLY
1	C	382	THR
1	C	414	ALA
1	C	534	TYR
1	A	301	GLY
1	A	338	ASP
1	C	14	ALA
1	C	210	ALA
1	C	52	GLY
1	C	266	PRO
1	C	89	PRO
1	C	110	PRO

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	463/478 (97%)	430 (93%)	33 (7%)	14 46
1	C	450/478 (94%)	410 (91%)	40 (9%)	9 35
All	All	913/956 (96%)	840 (92%)	73 (8%)	12 40

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	31	SER
1	A	45	MET
1	A	51	LEU
1	A	96	VAL
1	A	119	TYR
1	A	134	ARG
1	A	164	THR
1	A	192	PHE
1	A	203	ASP
1	A	216	LYS
1	A	229	ARG
1	A	246	LEU
1	A	251	THR
1	A	279	VAL
1	A	292	PHE
1	A	293	LYS
1	A	294	ASN
1	A	302	VAL
1	A	313	TYR
1	A	315	THR
1	A	317	ASP
1	A	352	VAL
1	A	376	ASP
1	A	382	THR
1	A	412	MET
1	A	426	ILE

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Mol	Chain	Res	Type
1	A	439	THR
1	A	468	LEU
1	A	475	GLU
1	A	476	ILE
1	A	495	GLN
1	A	558	THR
1	C	1	MET
1	C	24	CYS
1	C	28	VAL
1	C	45	MET
1	C	51	LEU
1	C	98	GLN
1	C	119	TYR
1	C	129	HIS
1	C	134	ARG
1	C	168	MET
1	C	178	GLN
1	C	179	GLU
1	C	180	ASN
1	C	184	MET
1	C	185	GLU
1	C	189	LEU
1	C	209	ARG
1	C	212	ASN
1	C	214	VAL
1	C	222	GLU
1	C	223	TYR
1	C	227	MET
1	C	234	ILE
1	C	260	LEU
1	C	272	LEU
1	C	308	ASP
1	C	358	VAL
1	C	362	VAL
1	C	387	THR
1	C	453	GLU
1	C	468	LEU
1	C	470	VAL
1	C	480	GLN
1	C	508	THR
1	C	513	GLU
1	C	523	LEU

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Mol	Chain	Res	Type
1	C	536	HIS
1	C	537	CYS
1	C	540	LEU
1	C	558	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	HIS
1	A	366	HIS
1	C	97	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	61/77 (79%)	15 (24%)	2 (3%)
2	D	62/77 (80%)	17 (27%)	2 (3%)
All	All	123/154 (79%)	32 (26%)	4 (3%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	914	A
2	B	917	U
2	B	918	G
2	B	919	G
2	B	923	G
2	B	929	C
2	B	947	G
2	B	949	U
2	B	957	C
2	B	959	A
2	B	960	A
2	B	962	C
2	B	963	C
2	B	973	C
2	B	974	G
2	D	902	C
2	D	917	U
2	D	918	G

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Mol	Chain	Res	Type
2	D	919	G
2	D	923	G
2	D	924	A
2	D	941	C
2	D	947	G
2	D	949	U
2	D	957	C
2	D	959	A
2	D	960	A
2	D	962	C
2	D	963	C
2	D	973	C
2	D	974	G
2	D	975	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	958	G
2	B	962	C
2	D	958	G
2	D	962	C

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)

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 (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	563/586 (96%)	-0.35	5 (0%)	84	63	69, 118, 178, 217	0
1	C	553/586 (94%)	-0.38	5 (0%)	84	63	71, 117, 177, 218	0
2	B	63/77 (81%)	-0.49	0	100	100	83, 125, 213, 258	0
2	D	64/77 (83%)	-0.52	0	100	100	91, 124, 235, 254	0
All	All	1243/1326 (93%)	-0.38	10 (0%)	86	65	69, 119, 182, 258	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	300	MET	3.2
1	C	181	ALA	3.1
1	A	222	GLU	3.0
1	A	296	GLU	2.9
1	C	13	GLN	2.6
1	A	217	LEU	2.2
1	C	299	PRO	2.2
1	A	385	GLY	2.1
1	A	200	TYR	2.1
1	C	180	ASN	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.