



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QTQ
Title : GLUTAMINYL-TRNA SYNTHETASE COMPLEXED WITH TRNA AND
AN AMINO ACID ANALOG
Authors : Rath, V.L.; Silvan, L.F.; Beijer, B.; Sproat, B.S.; Steitz, T.A.
Deposited on : 1998-01-28
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

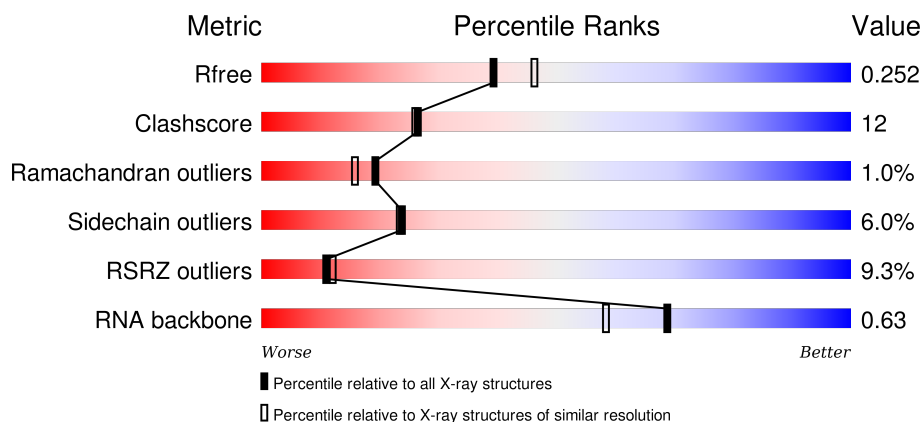
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)
RNA backbone	2183	1002 (2.80-1.74)

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. 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	B	75	<div> <div>9%</div> <div>41%</div> <div>47%</div> <div>11%</div> <div>.</div> </div>
2	A	553	<div> <div>9%</div> <div>71%</div> <div>22%</div> <div>.</div> <div>.</div> </div>

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
3	SO4	A	1396	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6061 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.

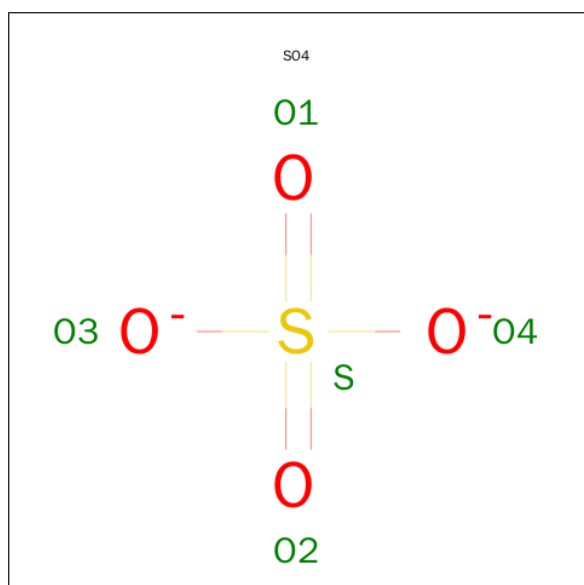
- Molecule 1 is a RNA chain called RNA (TRNA GLN II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	74	Total	C	N	O	P	0	0	0
			1570	702	279	516	73			

- Molecule 2 is a protein called PROTEIN (GLUTAMINYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4279	2704	752	802	21			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



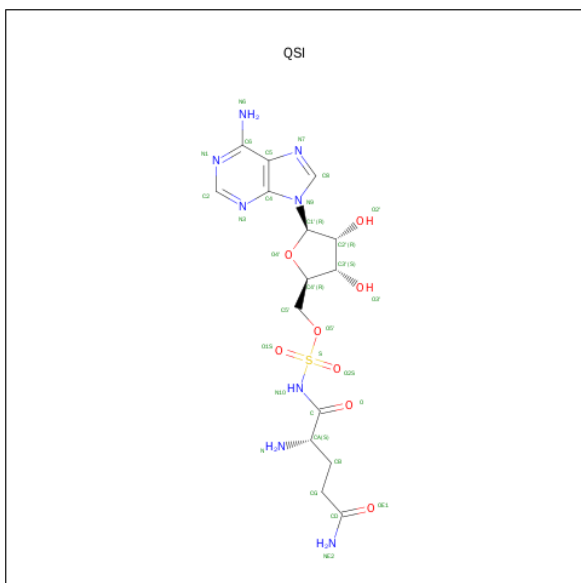
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE (three-letter code: QSI) (formula: C₁₅H₂₂N₈O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	15	8	8	1		

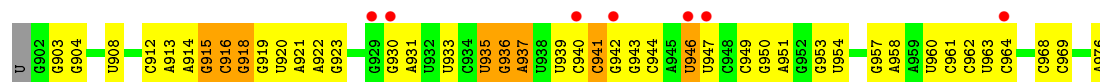
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	0
			135	135		
5	B	25	Total	O	0	0
			25	25		

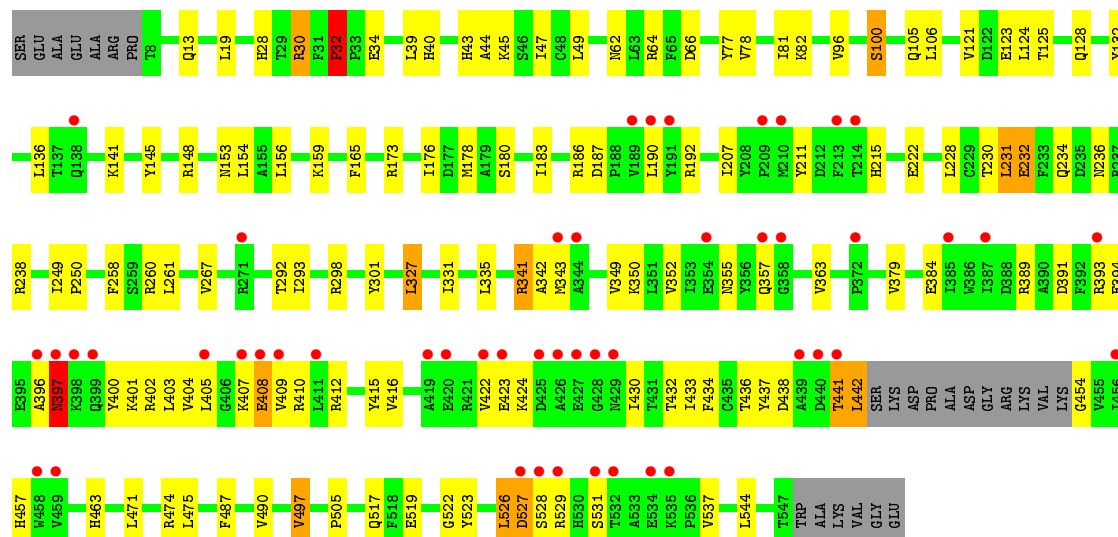
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: RNA (TRNA GLN II)



- Molecule 2: PROTEIN (GLUTAMINYL-TRNA SYNTHETASE)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	238.78 Å 93.36 Å 115.26 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25 28.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	83.6 (30.00-2.25) 83.7 (28.00-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.24 Å)	Xtriage
Refinement program	X-PLOR 0.3	Depositor
R, R_{free}	0.244 , 0.254 0.242 , 0.252	Depositor DCC
R_{free} test set	5205 reflections (10.13%)	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 51377 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6061	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: QSI, SO4

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	B	0.35	0/1753	0.67	0/2730
2	A	0.36	0/4379	0.60	1/5928 (0.0%)
All	All	0.35	0/6132	0.62	1/8658 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	396	ALA	N-CA-C	7.32	130.76	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	915	G	Sidechain

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	B	1570	0	801	44	0
2	A	4279	0	4172	91	0
3	A	20	0	0	1	0
4	A	32	0	22	1	0
5	A	135	0	0	2	0
5	B	25	0	0	0	0
All	All	6061	0	4995	133	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 12.

All (133) 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:919:G:H1'	1:B:920:U:H5	1.28	0.99
1:B:946:U:H4'	1:B:947:U:C5	1.98	0.98
1:B:919:G:H1'	1:B:920:U:C5	2.10	0.85
1:B:960:U:H5''	1:B:961:C:H5	1.43	0.84
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.60	0.84
2:A:123:GLU:HG2	2:A:148:ARG:HH22	1.44	0.81
1:B:903:G:O2'	1:B:904:G:H5'	1.86	0.76
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.71	0.72
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.72	0.70
2:A:529:ARG:HA	2:A:529:ARG:HE	1.56	0.70
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.72	0.70
1:B:930:G:O2'	1:B:931:A:H5'	1.92	0.68
2:A:517:GLN:HG3	2:A:523:TYR:CE1	2.28	0.68
2:A:30:ARG:NH1	2:A:32:PRO:HG3	2.08	0.68
2:A:355:ASN:HB2	2:A:436:THR:HG22	1.78	0.65
2:A:100:SER:HB2	5:A:1065:HOH:O	1.99	0.63
2:A:121:VAL:H	2:A:153:ASN:ND2	1.97	0.63
1:B:946:U:H4'	1:B:947:U:C6	2.33	0.62
1:B:960:U:H5''	1:B:961:C:C5	2.31	0.62
1:B:963:U:H2'	1:B:964:C:C6	2.34	0.62
2:A:407:LYS:HG3	2:A:408:GLU:H	1.64	0.62
1:B:940:C:H2'	1:B:941:C:C6	2.34	0.62
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.81	0.62
2:A:232:GLU:HG3	5:A:1053:HOH:O	1.99	0.62
1:B:914:A:H2'	1:B:915:G:H5'	1.82	0.62
2:A:531:SER:HB3	2:A:537:VAL:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.82	0.60
2:A:40:HIS:HA	2:A:292:THR:HA	1.83	0.60
2:A:526:LEU:HG	2:A:527:ASP:H	1.67	0.59
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.50	0.59
2:A:39:LEU:CD1	2:A:81:ILE:HG12	2.33	0.59
1:B:914:A:C2'	1:B:915:G:H5'	2.34	0.58
2:A:401:LYS:O	2:A:454:GLY:HA3	2.06	0.56
2:A:125:THR:HG23	2:A:128:GLN:HE21	1.70	0.56
2:A:407:LYS:HG3	2:A:408:GLU:N	2.21	0.56
2:A:410:ARG:HD3	2:A:416:VAL:HG22	1.89	0.55
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.42	0.55
1:B:943:G:O2'	1:B:944:C:H5'	2.06	0.55
1:B:957:G:H2'	1:B:958:A:H5'	1.88	0.55
2:A:487:PHE:O	2:A:490:VAL:HG12	2.07	0.54
1:B:916:C:H4'	1:B:918:G:OP2	2.08	0.54
2:A:32:PRO:HA	2:A:64:ARG:O	2.08	0.54
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.43	0.54
1:B:976:A:H4'	2:A:34:GLU:OE1	2.07	0.54
2:A:236:ASN:HD22	2:A:236:ASN:H	1.57	0.53
1:B:931:A:C2	1:B:940:C:H1'	2.44	0.53
2:A:527:ASP:C	2:A:529:ARG:H	2.11	0.53
2:A:123:GLU:HG2	2:A:148:ARG:NH2	2.19	0.53
1:B:919:G:O3'	1:B:920:U:H6	1.91	0.52
2:A:522:GLY:HA2	2:A:544:LEU:CD1	2.39	0.52
1:B:953:G:O2'	1:B:954:U:H5'	2.10	0.51
2:A:415:TYR:CE1	2:A:442:LEU:HD22	2.46	0.51
1:B:961:C:H2'	1:B:962:C:H6	1.75	0.51
2:A:173:ARG:HD2	2:A:187:ASP:O	2.11	0.51
2:A:341:ARG:H	2:A:341:ARG:HD2	1.77	0.50
2:A:123:GLU:CG	2:A:148:ARG:HH22	2.20	0.50
1:B:908:U:H5'	1:B:949:C:OP2	2.11	0.50
2:A:531:SER:CB	2:A:537:VAL:H	2.25	0.50
1:B:939:U:H2'	1:B:940:C:O4'	2.12	0.49
2:A:423:GLU:HB2	2:A:434:PHE:HE1	1.77	0.49
2:A:438:ASP:HB3	2:A:441:THR:OG1	2.13	0.49
2:A:249:ILE:HG13	2:A:250:PRO:HD2	1.95	0.49
1:B:933:U:H2'	1:B:935:U:OP1	2.11	0.49
2:A:424:LYS:HA	2:A:430:ILE:HA	1.94	0.49
2:A:43:HIS:O	2:A:47:ILE:HG13	2.12	0.49
2:A:403:LEU:N	2:A:409:VAL:HG11	2.27	0.49
2:A:397:ASN:HD22	2:A:400:TYR:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:393:ARG:O	2:A:404:VAL:HA	2.13	0.49
2:A:145:TYR:O	2:A:148:ARG:HG3	2.12	0.48
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.48	0.48
2:A:123:GLU:HB2	2:A:145:TYR:CE2	2.48	0.48
2:A:77:TYR:O	2:A:81:ILE:HG13	2.14	0.48
2:A:394:GLU:HA	2:A:405:LEU:HB2	1.95	0.48
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.44	0.48
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.96	0.48
1:B:962:C:H2'	1:B:963:U:C6	2.49	0.47
2:A:211:TYR:CE1	4:A:998:QSI:HG1	2.50	0.47
2:A:82:LYS:HD3	2:A:96:VAL:HG21	1.96	0.47
2:A:442:LEU:HD23	2:A:442:LEU:N	2.30	0.47
1:B:961:C:H2'	1:B:962:C:C6	2.50	0.47
2:A:123:GLU:HB2	2:A:145:TYR:CZ	2.50	0.46
1:B:908:U:C2	1:B:915:G:O6	2.68	0.46
1:B:950:G:O2'	1:B:951:A:H5'	2.15	0.46
1:B:908:U:H2'	1:B:913:A:N6	2.31	0.46
2:A:341:ARG:N	2:A:341:ARG:HD2	2.31	0.46
1:B:912:C:C2'	1:B:913:A:H5'	2.47	0.45
2:A:230:THR:HA	2:A:258:PHE:O	2.16	0.45
1:B:916:C:O5'	1:B:916:C:O2	2.34	0.45
2:A:64:ARG:HD3	2:A:222:GLU:OE2	2.17	0.45
1:B:936:G:H3'	1:B:937:A:C5'	2.45	0.45
2:A:230:THR:HG21	2:A:260:ARG:HB3	1.99	0.45
1:B:936:G:H3'	1:B:937:A:H5'	1.99	0.45
2:A:125:THR:HG23	2:A:128:GLN:NE2	2.32	0.45
2:A:343:MET:HE1	2:A:457:HIS:HA	1.99	0.45
1:B:939:U:O2'	1:B:940:C:H5'	2.16	0.45
2:A:331:ILE:HG13	2:A:335:LEU:HD22	2.00	0.44
1:B:922:A:H2'	1:B:923:G:O4'	2.17	0.44
1:B:919:G:C4	1:B:957:G:N2	2.86	0.44
2:A:44:ALA:HB2	2:A:293:ILE:HD11	2.00	0.44
2:A:363:VAL:HG22	2:A:379:VAL:O	2.18	0.44
2:A:178:MET:O	2:A:186:ARG:HD2	2.18	0.43
2:A:474:ARG:HB3	2:A:474:ARG:HE	1.67	0.43
2:A:531:SER:HA	2:A:537:VAL:HG23	2.01	0.43
2:A:463:HIS:O	2:A:505:PRO:HD3	2.19	0.43
2:A:238:ARG:N	2:A:238:ARG:HD2	2.34	0.43
2:A:416:VAL:HG23	2:A:441:THR:HB	2.02	0.42
2:A:180:SER:O	2:A:186:ARG:NH1	2.52	0.42
1:B:908:U:H2'	1:B:913:A:H61	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:LYS:HD2	2:A:261:LEU:HB2	2.02	0.42
2:A:298:ARG:HG3	2:A:527:ASP:OD2	2.20	0.42
1:B:935:U:C5	1:B:937:A:C2	3.08	0.42
1:B:903:G:C2'	1:B:904:G:H5'	2.48	0.41
2:A:526:LEU:O	2:A:527:ASP:HB3	2.20	0.41
2:A:433:ILE:N	2:A:433:ILE:HD12	2.34	0.41
2:A:350:LYS:O	2:A:432:THR:HA	2.19	0.41
1:B:941:C:H2'	1:B:942:G:H8	1.85	0.41
2:A:28:HIS:HE1	2:A:62:ASN:OD1	2.03	0.41
2:A:30:ARG:NH2	2:A:228:LEU:O	2.54	0.41
1:B:916:C:HO2'	1:B:918:G:P	2.44	0.41
2:A:301:TYR:CE2	2:A:331:ILE:HB	2.56	0.41
2:A:422:VAL:HG22	2:A:423:GLU:N	2.36	0.41
2:A:522:GLY:CA	2:A:544:LEU:HD13	2.45	0.41
2:A:342:ALA:O	2:A:519:GLU:HB2	2.20	0.41
1:B:912:C:H2'	1:B:913:A:H5'	2.03	0.41
1:B:916:C:O2'	1:B:918:G:P	2.79	0.41
2:A:301:TYR:HE2	2:A:327:LEU:HD22	1.85	0.41
2:A:517:GLN:HG3	2:A:523:TYR:CD1	2.56	0.40
1:B:916:C:N4	2:A:13:GLN:HE22	2.19	0.40
2:A:267:VAL:HB	3:A:1395:SO4:O1	2.20	0.40
2:A:207:ILE:O	2:A:207:ILE:HG13	2.20	0.40
2:A:349:VAL:HB	2:A:389:ARG:HG2	2.03	0.40
2:A:231:LEU:O	2:A:234:GLN:HG3	2.22	0.40
1:B:968:C:H2'	1:B:969:C:H6	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	A	525/553 (95%)	501 (95%)	19 (4%)	5 (1%)	19	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	397	ASN
2	A	527	ASP
2	A	32	PRO
2	A	526	LEU
2	A	176	ILE

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	
2	A	463/481 (96%)	435 (94%)	28 (6%)	24	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	19	LEU
2	A	30	ARG
2	A	32	PRO
2	A	49	LEU
2	A	66	ASP
2	A	78	VAL
2	A	100	SER
2	A	105	GLN
2	A	106	LEU
2	A	124	LEU
2	A	154	LEU
2	A	156	LEU
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	232	GLU
2	A	327	LEU
2	A	341	ARG
2	A	357	GLN
2	A	397	ASN

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Mol	Chain	Res	Type
2	A	408	GLU
2	A	412	ARG
2	A	437	TYR
2	A	441	THR
2	A	442	LEU
2	A	475	LEU
2	A	497	VAL
2	A	528	SER

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

Mol	Chain	Res	Type
2	A	28	HIS
2	A	107	HIS
2	A	115	ASN
2	A	128	GLN
2	A	142	ASN
2	A	153	ASN
2	A	226	HIS
2	A	236	ASN
2	A	318	GLN
2	A	355	ASN
2	A	368	HIS
2	A	397	ASN
2	A	457	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/75 (97%)	7 (9%)	1 (1%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	918	G
1	B	921	A
1	B	935	U
1	B	936	G
1	B	937	A
1	B	941	C

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Mol	Chain	Res	Type
1	B	946	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	916	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	SO4	A	1393	-	4,4,4	0.18	0	6,6,6	0.09	0
3	SO4	A	1394	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	A	1395	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	1396	-	4,4,4	0.23	0	6,6,6	0.07	0
4	QSI	A	998	-	27,34,34	1.49	3 (11%)	33,50,50	1.31	3 (9%)

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
3	SO4	A	1393	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
4	QSI	A	998	-	-	0/18/40/40	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	QSI	C-N10	-2.00	1.34	1.37
4	A	998	QSI	O2S-S	4.54	1.46	1.42
4	A	998	QSI	O1S-S	4.84	1.46	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	QSI	O2S-S-O1S	-5.77	113.86	120.77
4	A	998	QSI	O-C-CA	2.20	125.32	119.80
4	A	998	QSI	O5'-C5'-C4'	2.38	112.47	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1395	SO4	1	0
4	A	998	QSI	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

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	B	74/75 (98%)	0.46	7 (9%) 10 11	24, 59, 89, 99	0
2	A	529/553 (95%)	0.31	49 (9%) 11 12	17, 39, 86, 98	0
All	All	603/628 (96%)	0.33	56 (9%) 11 12	17, 40, 88, 99	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	947	U	7.6
1	B	946	U	7.1
2	A	397	ASN	5.4
2	A	426	ALA	5.3
2	A	439	ALA	5.3
2	A	399	GLN	4.5
2	A	411	LEU	4.0
2	A	427	GLU	3.7
2	A	458	TRP	3.4
2	A	534	GLU	3.3
2	A	398	LYS	3.3
2	A	456	ILE	3.2
2	A	528	SER	3.2
2	A	429	ASN	3.2
2	A	420	GLU	3.0
2	A	405	LEU	3.0
2	A	527	ASP	2.9
2	A	440	ASP	2.9
2	A	385	ILE	2.8
2	A	191	TYR	2.8
2	A	209	PRO	2.7
2	A	396	ALA	2.6
2	A	425	ASP	2.6
2	A	407	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	354	GLU	2.5
2	A	441	THR	2.5
2	A	422	VAL	2.5
2	A	387	ILE	2.5
2	A	409	VAL	2.5
2	A	419	ALA	2.4
2	A	344	ALA	2.4
2	A	138	GLN	2.4
2	A	210	MET	2.4
2	A	357	GLN	2.4
2	A	535	LYS	2.4
2	A	190	LEU	2.3
1	B	929	G	2.3
2	A	271	ARG	2.3
2	A	372	PRO	2.3
2	A	213	PHE	2.3
2	A	358	GLY	2.3
1	B	964	C	2.3
1	B	942	G	2.3
2	A	214	THR	2.3
2	A	428	GLY	2.3
2	A	529	ARG	2.3
2	A	343	MET	2.3
2	A	408	GLU	2.3
2	A	189	VAL	2.2
2	A	393	ARG	2.1
2	A	459	VAL	2.1
1	B	940	C	2.1
2	A	532	THR	2.1
1	B	930	G	2.1
2	A	423	GLU	2.1
2	A	531	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	1396	5/5	0.81	0.16	3.91	87,93,98,98	0
3	SO4	A	1395	5/5	0.95	0.15	1.08	90,92,96,97	0
4	QSI	A	998	32/32	0.96	0.20	0.37	28,40,50,54	0
3	SO4	A	1394	5/5	0.97	0.19	0.09	64,66,70,72	0
3	SO4	A	1393	5/5	0.87	0.26	-	84,84,89,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.