



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3QSY
Title : Recognition of the methionylated initiator tRNA by the translation initiation factor 2 in Archaea
Authors : Nikonov, O.S.; Stolboushkina, E.A.; Zelinskaya, N.V.; Nikulin, A.D.; Garber, M.B.; Nikonov, S.V.
Deposited on : 2011-02-22
Resolution : 3.20 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

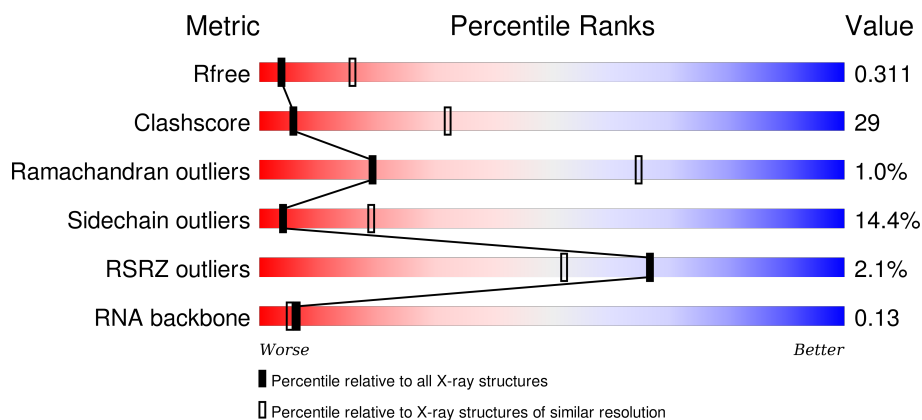
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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 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	A	415	<div> <div>2%</div> <div>42%</div> <div>51%</div> <div>7%</div> </div>
2	B	89	<div> <div>3%</div> <div>52%</div> <div>37%</div> <div>11%</div> </div>
3	D	77	<div> <div>8%</div> <div>42%</div> <div>45%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5593 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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3220	2063	549	595	13			

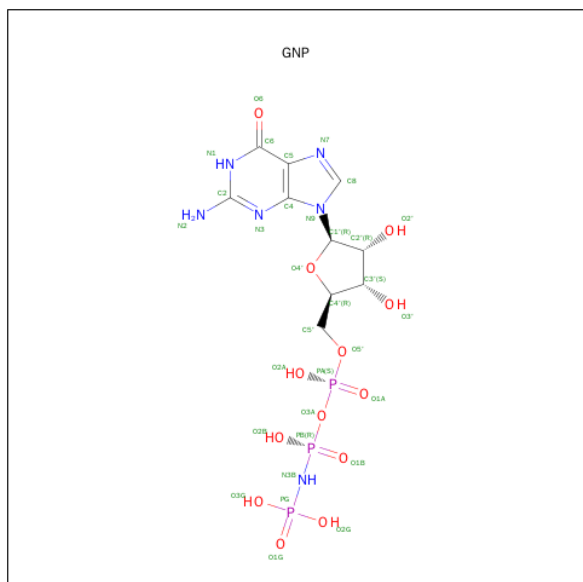
- Molecule 2 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			694	439	116	138	1			

- Molecule 3 is a RNA chain called tRNA.

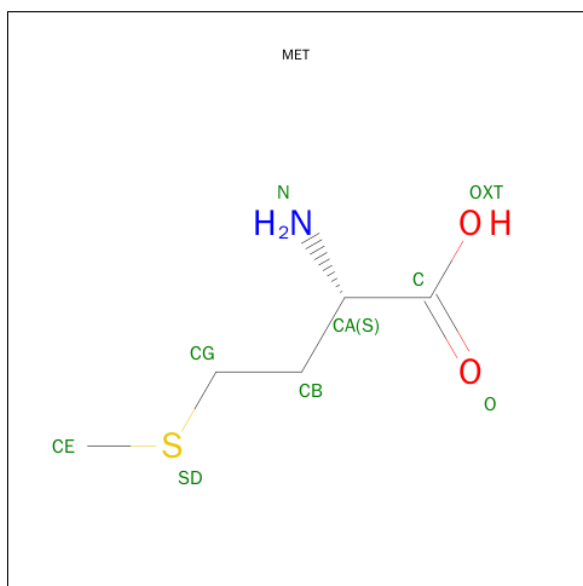
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).

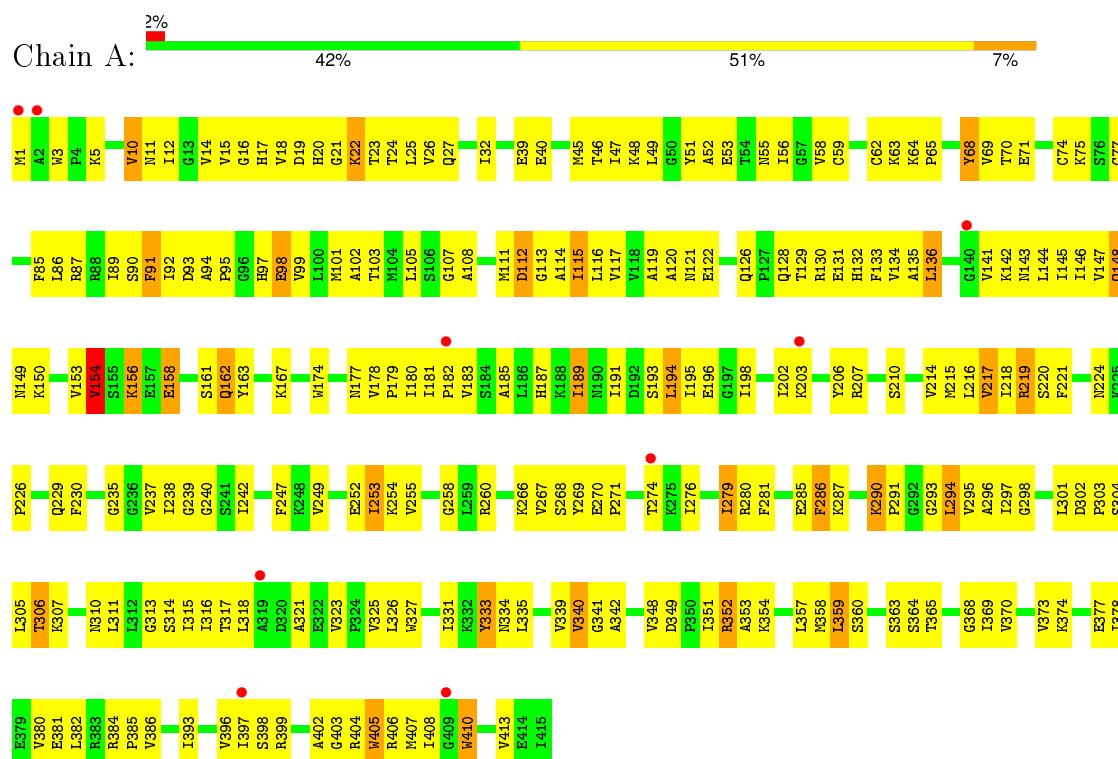


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

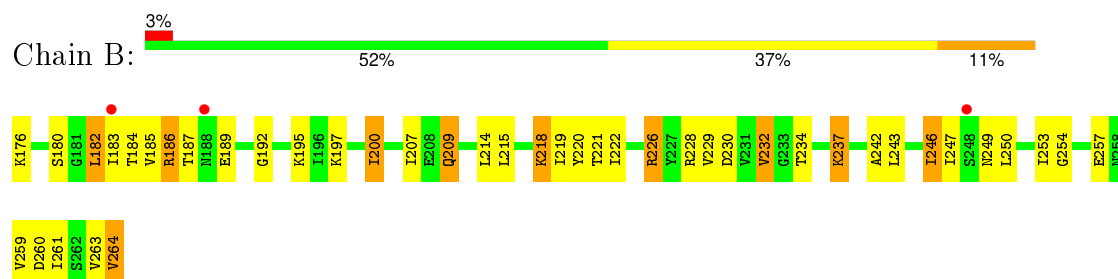
3 Residue-property plots

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.

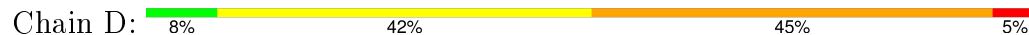
- Molecule 1: Translation initiation factor 2 subunit gamma



- Molecule 2: Translation initiation factor 2 subunit alpha



- Molecule 3: tRNA



U60	C1	U61	C2	U62	C3	U63	C4	U64	C5	U65	C6	U66	C7	U67	C8	U68	C9	U69	C10	U70	C11	U71	C12	U72	C13	U73	C14	U74	C15	U75	C16	U76	C17	U77A	C18	U78	C19	U79	C20	U80	C21	U81	C22	U82	C23	U83	C24	U84	C25	U85	C26	U86	C27	U87	C28	U88	C29	U89	C30	U90	C31	U91	C32	U92	C33	U93	C34	U94	C35	U95	C36	U96	C37	U97	C38	U98	C39	U99	C40	U100	C41	U101	C42	U102	C43	U103	C44	U104	C45	U105	C46	U106	C47	U107	C48	U108	C49	U109	C50	U110	C51	U111	C52	U112	C53	U113	C54	U114	C55	U115	C56	U116	C57	U117	C58	U118	C59	U119	C60	U120	C61	U121	C62	U122	C63	U123	C64	U124	C65	U125	C66	U126	C67	U127	C68	U128	C69	U129	C70	U130	C71	U131	C72	U132	C73	U133	C74	U134	C75	U135	C76	U136	C77	U137	C78	U138	C79	U139	C80	U140	C81	U141	C82	U142	C83	U143	C84	U144	C85	U145	C86	U146	C87	U147	C88	U148	C89	U149	C90	U150	C91	U151	C92	U152	C93	U153	C94	U154	C95	U155	C96	U156	C97	U157	C98	U158	C99	U159	C100	U160
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.68Å 93.68Å 220.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.95 – 3.20 14.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (14.95-3.20) 100.0 (14.95-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.278 , 0.302 0.293 , 0.311	Depositor DCC
R_{free} test set	973 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	1.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , 130.8	EDS
Estimated twinning fraction	0.500 for -h,-k,l 0.470 for -h,-k,l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18940 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GNP

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	0.36	0/3279	0.68	0/4440
2	B	0.32	0/699	0.63	0/942
3	D	0.54	0/1831	1.08	7/2853 (0.2%)
All	All	0.42	0/5809	0.84	7/8235 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	61	C	N1-C2-O2	5.65	122.29	118.90
3	D	68	C	N1-C2-O2	5.63	122.28	118.90
3	D	30	G	N3-C4-C5	-5.62	125.79	128.60
3	D	61	C	C5-C6-N1	5.42	123.71	121.00
3	D	30	G	N3-C4-N9	5.12	129.07	126.00
3	D	6	G	N3-C4-N9	5.09	129.06	126.00
3	D	15	G	C4-N9-C1'	5.07	133.09	126.50

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	3220	0	3344	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	694	0	734	33	0
3	D	1639	0	836	61	0
4	A	32	0	13	6	0
5	D	8	0	8	5	0
All	All	5593	0	4935	302	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 29.

All (302) 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:281:PHE:HB2	1:A:286:PHE:HB2	1.56	0.88
1:A:128:GLN:HA	1:A:131:GLU:HB3	1.56	0.85
1:A:130:ARG:HH22	1:A:340:VAL:HB	1.40	0.85
1:A:146:ILE:O	1:A:180:ILE:HA	1.75	0.85
1:A:99:VAL:HG11	3:D:71:C:H5'	1.59	0.84
1:A:215:MET:HB2	1:A:242:ILE:HG13	1.61	0.83
1:A:183:VAL:HG11	1:A:194:LEU:HB3	1.60	0.81
2:B:254:GLY:HA2	2:B:259:VAL:H	1.47	0.79
1:A:249:VAL:HG22	1:A:287:LYS:HB3	1.64	0.79
1:A:237:VAL:HG12	1:A:298:GLY:HA2	1.65	0.78
1:A:370:VAL:HG13	1:A:378:ILE:HG21	1.66	0.78
1:A:307:LYS:HG3	1:A:310:ASN:HB3	1.67	0.77
2:B:207:ILE:HD12	2:B:249:ASN:HD21	1.49	0.77
1:A:226:PRO:HB2	2:B:220:TYR:HA	1.67	0.76
1:A:55:ASN:HB3	1:A:70:THR:HG23	1.68	0.74
1:A:219:ARG:HH21	1:A:220:SER:HA	1.54	0.73
1:A:181:ILE:HG21	1:A:194:LEU:HA	1.71	0.73
1:A:352:ARG:HD3	1:A:353:ALA:H	1.54	0.72
1:A:224:ASN:HD21	3:D:2:G:H4'	1.55	0.72
2:B:184:THR:HB	2:B:263:VAL:HA	1.71	0.72
1:A:281:PHE:H	1:A:285:GLU:HA	1.52	0.72
1:A:230:PHE:HB3	2:B:219:ILE:HB	1.73	0.71
1:A:365:THR:HG22	3:D:73:A:H61	1.58	0.69
1:A:217:VAL:HA	1:A:240:GLY:HA3	1.73	0.69
3:D:19:G:H22	3:D:56:C:H2'	1.58	0.69
2:B:226:ARG:NH1	3:D:17:C:OP2	2.26	0.68
1:A:147:VAL:HG22	1:A:181:ILE:HD12	1.75	0.68
3:D:22:G:O2'	3:D:23:C:H5'	1.94	0.68
1:A:357:LEU:CD2	1:A:408:ILE:HD11	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HH11	1:A:353:ALA:H	1.41	0.68
1:A:26:VAL:HG11	1:A:93:ASP:HB2	1.74	0.67
1:A:25:LEU:HD21	1:A:115:ILE:HD13	1.77	0.67
3:D:23:C:H2'	3:D:24:U:C6	2.30	0.67
1:A:108:ALA:HA	1:A:111:MET:HB3	1.77	0.66
1:A:229:GLN:HG2	2:B:218:LYS:HB3	1.76	0.66
1:A:94:ALA:HB2	1:A:107:GLY:HA3	1.76	0.66
1:A:194:LEU:C	1:A:194:LEU:HD12	2.16	0.66
2:B:187:THR:HG22	2:B:259:VAL:HG22	1.78	0.66
2:B:192:GLY:HA2	2:B:195:LYS:HB2	1.76	0.66
3:D:69:C:H2'	3:D:70:G:H4'	1.77	0.65
1:A:97:HIS:N	1:A:128:GLN:HE22	1.95	0.65
3:D:40:C:C6	3:D:40:C:H5''	2.31	0.65
1:A:276:ILE:HG21	1:A:279:ILE:HD11	1.78	0.65
1:A:14:VAL:HG22	1:A:22:LYS:HG3	1.79	0.64
1:A:113:GLY:HA3	1:A:143:ASN:HD22	1.62	0.64
3:D:27:U:H3	3:D:43:A:N6	1.95	0.64
1:A:130:ARG:HH12	1:A:340:VAL:HG21	1.60	0.64
2:B:250:LEU:HB2	2:B:261:ILE:HD12	1.80	0.64
3:D:27:U:H3	3:D:43:A:H61	1.47	0.63
1:A:269:TYR:H	1:A:385:PRO:HG2	1.63	0.63
1:A:195:ILE:HA	1:A:198:ILE:CG1	2.28	0.63
1:A:191:ILE:HG23	1:A:194:LEU:CD2	2.29	0.63
2:B:263:VAL:HG22	2:B:264:VAL:HG22	1.81	0.62
1:A:280:ARG:HB3	1:A:296:ALA:H	1.64	0.62
1:A:191:ILE:HG23	1:A:194:LEU:HD23	1.81	0.62
1:A:17:HIS:HB3	1:A:20:HIS:CE1	2.34	0.62
1:A:220:SER:HB2	1:A:238:ILE:HG23	1.81	0.62
1:A:12:ILE:HG23	1:A:114:ALA:HA	1.80	0.62
1:A:218:ILE:HD12	1:A:219:ARG:HG3	1.82	0.62
2:B:207:ILE:HD11	2:B:246:ILE:HG22	1.82	0.61
3:D:63:G:H2'	3:D:64:G:C8	2.34	0.61
1:A:237:VAL:HG23	1:A:296:ALA:HB1	1.83	0.60
1:A:269:TYR:CE2	1:A:384:ARG:HD3	2.36	0.60
1:A:45:MET:HE1	3:D:71:C:C5	2.35	0.60
1:A:145:ILE:HG12	1:A:179:PRO:HD2	1.83	0.60
1:A:135:ALA:HA	3:D:74:C:C4	2.36	0.60
3:D:16:C:O2'	3:D:61:C:H5'	2.01	0.60
2:B:253:ILE:O	2:B:257:GLU:N	2.29	0.60
1:A:352:ARG:HH11	1:A:353:ALA:N	1.99	0.60
1:A:269:TYR:OH	1:A:384:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HG2	1:A:311:LEU:HG	1.84	0.59
1:A:360:SER:OG	1:A:396:VAL:HB	2.03	0.59
1:A:260:ARG:HH21	1:A:267:VAL:HG11	1.65	0.59
1:A:145:ILE:HG23	1:A:179:PRO:HB2	1.85	0.58
3:D:40:C:H6	3:D:40:C:H5''	1.68	0.58
2:B:250:LEU:O	2:B:254:GLY:N	2.33	0.58
3:D:10:G:N2	3:D:26:G:H1'	2.18	0.58
1:A:218:ILE:H	1:A:240:GLY:HA2	1.69	0.58
1:A:403:GLY:HA3	3:D:11:A:H2	1.68	0.57
1:A:368:GLY:HA2	1:A:381:GLU:O	2.04	0.57
1:A:342:ALA:N	1:A:406:ARG:HE	2.02	0.57
1:A:10:VAL:HG13	1:A:112:ASP:HB2	1.87	0.57
3:D:5:G:H2'	3:D:6:G:H4'	1.86	0.57
1:A:194:LEU:O	1:A:198:ILE:HG23	2.05	0.57
1:A:113:GLY:HA2	1:A:143:ASN:HB3	1.86	0.56
2:B:197:LYS:HA	2:B:200:ILE:HB	1.86	0.56
3:D:15:G:N2	3:D:16:C:H1'	2.20	0.56
1:A:11:ASN:HD22	1:A:89:ILE:HG23	1.71	0.56
1:A:323:VAL:H	1:A:326:LEU:HD11	1.71	0.56
1:A:95:PRO:O	1:A:103:THR:OG1	2.24	0.56
1:A:214:VAL:HG22	1:A:318:LEU:HD23	1.86	0.56
2:B:263:VAL:HG13	2:B:264:VAL:H	1.70	0.56
3:D:30:G:H2'	3:D:31:G:H4'	1.87	0.56
3:D:23:C:OP1	3:D:42:G:N1	2.38	0.55
1:A:117:VAL:HG22	1:A:147:VAL:HB	1.87	0.55
1:A:219:ARG:CZ	1:A:294:LEU:HB2	2.36	0.55
1:A:193:SER:HA	1:A:196:GLU:HG2	1.88	0.55
1:A:132:HIS:CE1	1:A:136:LEU:HD22	2.42	0.55
1:A:369:ILE:O	1:A:380:VAL:HA	2.07	0.55
1:A:147:VAL:HG13	1:A:181:ILE:HB	1.88	0.55
2:B:247:ILE:HG23	2:B:261:ILE:HD13	1.89	0.55
1:A:130:ARG:HG3	5:D:77:MET:CG	2.37	0.55
1:A:352:ARG:HD3	1:A:353:ALA:N	2.20	0.55
1:A:15:VAL:HG12	1:A:16:GLY:H	1.72	0.55
1:A:27:GLN:HG2	1:A:39:GLU:HB2	1.89	0.55
1:A:359:LEU:HD23	1:A:380:VAL:HG11	1.89	0.54
1:A:210:SER:HA	1:A:247:PHE:CZ	2.41	0.54
1:A:221:PHE:HE1	3:D:4:G:H5'	1.72	0.54
1:A:354:LYS:HB2	1:A:354:LYS:NZ	2.23	0.54
3:D:49:G:H2'	3:D:50:U:H5''	1.89	0.54
3:D:51:C:H2'	3:D:52:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ASN:O	2:B:253:ILE:HG12	2.08	0.54
1:A:214:VAL:HG11	1:A:317:THR:HA	1.89	0.54
1:A:302:ASP:O	1:A:304:SER:N	2.37	0.54
1:A:146:ILE:HG22	1:A:180:ILE:HG23	1.88	0.53
1:A:404:ARG:HG3	1:A:405:TRP:H	1.73	0.53
2:B:220:TYR:CE2	2:B:228:ARG:HB3	2.43	0.53
3:D:6:G:H1	3:D:67:C:H42	1.56	0.53
3:D:58:A:H2'	3:D:59:A:H5'	1.90	0.53
1:A:252:GLU:HB2	1:A:276:ILE:HD11	1.89	0.53
1:A:153:VAL:HG13	1:A:156:LYS:HE3	1.89	0.53
2:B:218:LYS:CG	2:B:230:ASP:HB3	2.39	0.53
1:A:339:VAL:HG21	1:A:348:VAL:HG23	1.90	0.53
1:A:116:LEU:HD22	1:A:144:LEU:HD12	1.90	0.53
1:A:280:ARG:HA	1:A:285:GLU:HB2	1.90	0.53
2:B:219:ILE:HG12	2:B:229:VAL:HG12	1.91	0.53
1:A:101:MET:HB2	1:A:128:GLN:NE2	2.24	0.52
1:A:195:ILE:HA	1:A:198:ILE:HG12	1.91	0.52
3:D:10:G:H2'	3:D:10:G:N3	2.24	0.52
1:A:163:TYR:OH	1:A:182:PRO:HD3	2.09	0.52
1:A:52:ALA:O	1:A:90:SER:HA	2.10	0.52
1:A:294:LEU:HD22	1:A:295:VAL:N	2.25	0.52
1:A:226:PRO:HD3	1:A:303:PRO:HB2	1.91	0.52
1:A:56:ILE:HG22	1:A:68:TYR:HE2	1.75	0.52
1:A:21:GLY:HA3	1:A:149:ASN:HD22	1.75	0.52
1:A:187:HIS:C	1:A:189:ILE:H	2.13	0.52
1:A:130:ARG:NH1	1:A:340:VAL:HG21	2.25	0.52
1:A:358:MET:HB3	1:A:398:SER:HB3	1.92	0.52
1:A:253:ILE:HA	1:A:274:THR:O	2.10	0.52
1:A:402:ALA:HB1	3:D:25:C:H4'	1.92	0.51
1:A:359:LEU:HB3	1:A:382:LEU:HD11	1.91	0.51
3:D:8:U:C2	3:D:15:G:H8	2.28	0.51
1:A:133:PHE:HE1	1:A:174:TRP:HE1	1.58	0.51
3:D:28:C:N4	3:D:29:G:O6	2.43	0.51
1:A:335:LEU:HA	1:A:410:TRP:H	1.76	0.51
1:A:301:LEU:HD22	1:A:305:LEU:HB2	1.92	0.51
1:A:358:MET:O	1:A:397:ILE:HA	2.11	0.51
2:B:185:VAL:HG22	2:B:261:ILE:HG13	1.93	0.51
1:A:22:LYS:HD2	4:A:501:GNP:HNB3	1.76	0.51
2:B:186:ARG:HD3	2:B:187:THR:N	2.26	0.50
1:A:149:ASN:HD21	1:A:185:ALA:HB3	1.76	0.50
1:A:14:VAL:HG11	1:A:25:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:G:N3	3:D:4:G:H2'	2.26	0.50
2:B:243:LEU:O	2:B:246:ILE:HG12	2.12	0.50
1:A:216:LEU:HD11	1:A:314:SER:O	2.12	0.50
1:A:56:ILE:HG22	1:A:68:TYR:CE2	2.46	0.50
1:A:23:THR:HG21	1:A:40:GLU:HB3	1.93	0.50
1:A:102:ALA:HA	3:D:74:C:OP1	2.12	0.50
1:A:26:VAL:HG12	1:A:91:PHE:CD1	2.47	0.49
1:A:255:VAL:O	1:A:271:PRO:HB3	2.12	0.49
3:D:36:U:N3	3:D:38:A:N1	2.60	0.49
1:A:130:ARG:HG3	5:D:77:MET:HG3	1.94	0.49
2:B:218:LYS:HG3	2:B:230:ASP:HB3	1.93	0.49
1:A:132:HIS:O	1:A:136:LEU:HB3	2.12	0.49
1:A:195:ILE:HA	1:A:198:ILE:HG13	1.94	0.49
1:A:258:GLY:O	1:A:269:TYR:HB3	2.12	0.49
1:A:142:LYS:HB2	1:A:202:ILE:HG12	1.93	0.49
1:A:239:GLY:CA	1:A:297:ILE:HG12	2.43	0.49
1:A:58:VAL:HG22	1:A:59:CYS:H	1.78	0.49
1:A:113:GLY:HA2	1:A:141:VAL:HG13	1.94	0.48
1:A:130:ARG:CZ	5:D:77:MET:HG2	2.43	0.48
1:A:235:GLY:O	1:A:301:LEU:N	2.45	0.48
1:A:129:THR:O	1:A:132:HIS:HB3	2.13	0.48
1:A:115:ILE:HD12	1:A:198:ILE:HG21	1.96	0.48
1:A:92:ILE:HG22	1:A:93:ASP:H	1.79	0.48
1:A:19:ASP:HA	4:A:501:GNP:PB	2.54	0.47
2:B:220:TYR:OH	2:B:230:ASP:HB2	2.14	0.47
1:A:334:ASN:HB2	1:A:410:TRP:CE2	2.48	0.47
1:A:71:GLU:CD	1:A:71:GLU:H	2.17	0.47
1:A:22:LYS:H	4:A:501:GNP:PB	2.36	0.47
1:A:150:LYS:HD2	4:A:501:GNP:C6	2.44	0.47
1:A:365:THR:HG22	3:D:73:A:N6	2.27	0.47
1:A:24:THR:HA	1:A:27:GLN:HE21	1.79	0.47
1:A:187:HIS:HB2	1:A:189:ILE:HG22	1.96	0.47
1:A:301:LEU:HD13	1:A:306:THR:HG22	1.96	0.47
1:A:325:VAL:HG23	1:A:327:TRP:CD1	2.49	0.47
2:B:215:LEU:HB2	2:B:232:VAL:HG23	1.96	0.47
1:A:154:VAL:HG21	1:A:158:GLU:HG3	1.97	0.47
1:A:99:VAL:HG22	3:D:72:A:H1'	1.97	0.47
1:A:101:MET:HG2	1:A:131:GLU:OE2	2.15	0.47
1:A:260:ARG:HE	1:A:267:VAL:HG21	1.78	0.47
3:D:62:C:H2'	3:D:63:G:C8	2.50	0.47
1:A:323:VAL:H	1:A:326:LEU:CD1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD12	1:A:217:VAL:H	1.80	0.47
2:B:182:LEU:HB2	2:B:222:ILE:HD11	1.95	0.47
1:A:280:ARG:HB3	1:A:296:ALA:N	2.29	0.47
3:D:6:G:O6	3:D:66:C:N4	2.48	0.47
3:D:44:A:H4'	3:D:45:G:OP1	2.15	0.46
1:A:115:ILE:HD11	1:A:147:VAL:HG21	1.97	0.46
3:D:3:C:H2'	3:D:4:G:C8	2.49	0.46
3:D:8:U:H5'	3:D:13:C:H41	1.80	0.46
1:A:315:ILE:HD11	1:A:364:SER:HB3	1.97	0.46
1:A:167:LYS:HA	1:A:167:LYS:HD3	1.54	0.46
1:A:341:GLY:HA2	1:A:406:ARG:HD2	1.98	0.46
1:A:113:GLY:CA	1:A:143:ASN:HB3	2.46	0.46
1:A:313:GLY:C	1:A:363:SER:HB3	2.37	0.46
1:A:126:GLN:HB2	1:A:129:THR:OG1	2.16	0.45
1:A:86:LEU:HG	1:A:87:ARG:HG2	1.98	0.45
2:B:176:LYS:N	2:B:234:THR:O	2.49	0.45
1:A:148:GLN:NE2	1:A:162:GLN:HE21	2.15	0.45
1:A:260:ARG:NH2	1:A:267:VAL:HG11	2.31	0.45
1:A:406:ARG:HD3	1:A:406:ARG:HA	1.75	0.45
1:A:321:ALA:HB3	1:A:326:LEU:HD13	1.98	0.45
1:A:17:HIS:NE2	1:A:122:GLU:OE2	2.48	0.45
1:A:49:LEU:HD12	1:A:49:LEU:H	1.82	0.45
1:A:398:SER:OG	1:A:399:ARG:N	2.50	0.45
1:A:26:VAL:HG12	1:A:91:PHE:CE1	2.52	0.45
1:A:218:ILE:N	1:A:240:GLY:HA2	2.31	0.45
1:A:331:ILE:HG12	1:A:413:VAL:HG22	1.97	0.45
3:D:57:A:H2'	3:D:58:A:H4'	1.98	0.45
1:A:407:MET:H	1:A:407:MET:HG3	1.61	0.45
1:A:12:ILE:HG13	1:A:112:ASP:O	2.17	0.44
1:A:351:ILE:HG21	1:A:373:VAL:HG13	1.98	0.44
1:A:146:ILE:HG13	1:A:178:VAL:HG11	2.00	0.44
1:A:370:VAL:HA	1:A:380:VAL:HG22	1.99	0.44
1:A:202:ILE:HD12	1:A:202:ILE:HA	1.81	0.44
1:A:128:GLN:O	1:A:132:HIS:HB2	2.16	0.44
1:A:287:LYS:HD3	1:A:287:LYS:HA	1.78	0.44
3:D:52:G:H2'	3:D:53:G:O4'	2.17	0.44
1:A:3:TRP:HE1	1:A:5:LYS:HE2	1.83	0.44
1:A:97:HIS:CD2	1:A:98:GLU:H	2.35	0.44
3:D:20:U:H2'	3:D:21:A:O5'	2.18	0.44
1:A:130:ARG:O	1:A:134:VAL:HG22	2.17	0.44
2:B:250:LEU:HD22	2:B:259:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:G:N2	3:D:5:G:C5	2.86	0.44
1:A:374:LYS:HA	1:A:374:LYS:HD3	1.81	0.44
1:A:130:ARG:NH1	5:D:77:MET:HG2	2.32	0.44
2:B:242:ALA:O	2:B:246:ILE:HG23	2.17	0.44
1:A:55:ASN:HA	1:A:85:PHE:CZ	2.53	0.44
1:A:268:SER:HA	1:A:385:PRO:HG2	2.00	0.44
2:B:209:GLN:HE21	2:B:209:GLN:HB2	1.61	0.44
1:A:305:LEU:H	1:A:305:LEU:HD12	1.83	0.44
1:A:75:LYS:HD2	1:A:75:LYS:HA	1.68	0.44
1:A:217:VAL:HG22	1:A:316:ILE:HG13	2.00	0.43
1:A:158:GLU:O	1:A:161:SER:HB2	2.18	0.43
5:D:77:MET:N	5:D:77:MET:SD	2.90	0.43
1:A:260:ARG:HG2	1:A:269:TYR:CE1	2.53	0.43
1:A:358:MET:HB3	1:A:398:SER:H	1.83	0.43
1:A:333:TYR:CD1	1:A:333:TYR:C	2.91	0.43
1:A:280:ARG:HA	1:A:285:GLU:CB	2.48	0.43
1:A:98:GLU:OE2	1:A:99:VAL:N	2.47	0.43
1:A:242:ILE:HG22	1:A:291:PRO:HG3	2.00	0.43
1:A:26:VAL:HA	1:A:91:PHE:CD2	2.53	0.43
1:A:270:GLU:HA	1:A:271:PRO:HD3	1.71	0.43
1:A:239:GLY:HA2	1:A:297:ILE:HG12	2.01	0.43
3:D:63:G:N1	3:D:64:G:C6	2.87	0.43
3:D:53:G:C6	3:D:54:U:C4	3.07	0.42
1:A:120:ALA:HA	1:A:162:GLN:HG3	2.00	0.42
1:A:150:LYS:HD2	4:A:501:GNP:C5	2.48	0.42
1:A:218:ILE:HD11	1:A:293:GLY:O	2.19	0.42
1:A:121:ASN:HD22	4:A:501:GNP:HN1	1.65	0.42
1:A:352:ARG:NH1	1:A:353:ALA:H	2.13	0.42
3:D:44:A:H3'	3:D:45:G:C5	2.54	0.42
3:D:50:U:C4	3:D:65:C:N3	2.88	0.42
1:A:403:GLY:HA3	3:D:11:A:C2	2.50	0.42
3:D:21:A:H2'	3:D:21:A:N3	2.34	0.42
1:A:333:TYR:C	1:A:333:TYR:HD1	2.23	0.42
1:A:307:LYS:CG	1:A:311:LEU:HG	2.48	0.42
1:A:20:HIS:NE2	1:A:119:ALA:HB2	2.34	0.42
1:A:63:LYS:N	1:A:63:LYS:HD2	2.34	0.42
1:A:249:VAL:HG13	1:A:287:LYS:O	2.19	0.42
1:A:239:GLY:HA3	1:A:297:ILE:HG12	2.02	0.42
1:A:325:VAL:HG23	1:A:327:TRP:NE1	2.34	0.42
1:A:15:VAL:HG12	1:A:16:GLY:N	2.35	0.41
3:D:65:C:H2'	3:D:66:C:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:A:C2'	3:D:59:A:H5'	2.49	0.41
1:A:242:ILE:H	1:A:291:PRO:HG3	1.84	0.41
1:A:219:ARG:C	1:A:219:ARG:HE	2.23	0.41
1:A:323:VAL:HB	1:A:326:LEU:HG	2.01	0.41
1:A:15:VAL:C	1:A:22:LYS:HZ2	2.24	0.41
1:A:253:ILE:HG22	1:A:254:LYS:HG3	2.01	0.41
3:D:30:G:H2'	3:D:31:G:C4'	2.50	0.41
1:A:64:LYS:N	1:A:65:PRO:HD2	2.35	0.41
1:A:97:HIS:O	1:A:128:GLN:NE2	2.53	0.41
3:D:5:G:H2'	3:D:6:G:C4'	2.51	0.41
1:A:281:PHE:CE1	1:A:290:LYS:HG2	2.56	0.41
1:A:132:HIS:CE1	1:A:136:LEU:HD13	2.56	0.41
1:A:22:LYS:NZ	1:A:117:VAL:HB	2.35	0.41
1:A:156:LYS:HA	1:A:156:LYS:HD2	1.91	0.41
1:A:195:ILE:O	1:A:198:ILE:HG13	2.21	0.41
3:D:62:C:H2'	3:D:63:G:O4'	2.20	0.41
1:A:105:LEU:HD22	1:A:105:LEU:H	1.86	0.41
1:A:14:VAL:HG11	1:A:25:LEU:HD23	2.03	0.40
1:A:217:VAL:HG23	1:A:314:SER:HB2	2.02	0.40
3:D:22:G:O2'	3:D:23:C:C5'	2.65	0.40
1:A:135:ALA:HA	3:D:74:C:C5	2.56	0.40
2:B:237:LYS:HD3	2:B:237:LYS:HA	1.86	0.40
1:A:281:PHE:HB2	1:A:286:PHE:CB	2.40	0.40
3:D:1:C:O5'	3:D:2:G:H5''	2.22	0.40
3:D:50:U:H3	3:D:64:G:N2	2.20	0.40
1:A:252:GLU:O	1:A:274:THR:O	2.40	0.40
3:D:43:A:C6	3:D:44:A:C5	3.10	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	
1	A	413/415 (100%)	331 (80%)	77 (19%)	5 (1%)	16	60
2	B	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
All	All	500/504 (99%)	406 (81%)	89 (18%)	5 (1%)	19	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	393	ILE
1	A	154	VAL
1	A	10	VAL
1	A	279	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	
1	A	357/357 (100%)	311 (87%)	46 (13%)	5	24
2	B	80/80 (100%)	64 (80%)	16 (20%)	1	8
All	All	437/437 (100%)	375 (86%)	62 (14%)	4	19

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	VAL
1	A	22	LYS
1	A	32	ILE
1	A	46	THR
1	A	48	LYS
1	A	51	TYR
1	A	53	GLU
1	A	62	CYS
1	A	68	TYR
1	A	69	VAL

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Mol	Chain	Res	Type
1	A	74	CYS
1	A	77	CYS
1	A	91	PHE
1	A	98	GLU
1	A	112	ASP
1	A	115	ILE
1	A	136	LEU
1	A	148	GLN
1	A	154	VAL
1	A	156	LYS
1	A	158	GLU
1	A	162	GLN
1	A	177	ASN
1	A	189	ILE
1	A	194	LEU
1	A	203	LYS
1	A	206	TYR
1	A	207	ARG
1	A	217	VAL
1	A	219	ARG
1	A	253	ILE
1	A	266	LYS
1	A	286	PHE
1	A	290	LYS
1	A	294	LEU
1	A	306	THR
1	A	333	TYR
1	A	340	VAL
1	A	349	ASP
1	A	352	ARG
1	A	359	LEU
1	A	377	GLU
1	A	386	VAL
1	A	405	TRP
1	A	410	TRP
2	B	180	SER
2	B	182	LEU
2	B	183	ILE
2	B	186	ARG
2	B	189	GLU
2	B	200	ILE
2	B	209	GLN

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Mol	Chain	Res	Type
2	B	214	LEU
2	B	218	LYS
2	B	221	THR
2	B	226	ARG
2	B	232	VAL
2	B	237	LYS
2	B	246	ILE
2	B	260	ASP
2	B	264	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	97	HIS
1	A	126	GLN
1	A	128	GLN
1	A	148	GLN
1	A	162	GLN
1	A	168	GLN
1	A	224	ASN
1	A	229	GLN
1	A	251	GLN
1	A	334	ASN
1	A	392	ASN
2	B	209	GLN
2	B	245	GLN
2	B	249	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	76/77 (98%)	52 (68%)	4 (5%)

All (52) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	2	G
3	D	3	C
3	D	6	G

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Mol	Chain	Res	Type
3	D	8	U
3	D	9	G
3	D	10	G
3	D	11	A
3	D	14	A
3	D	15	G
3	D	16	C
3	D	17	C
3	D	18	G
3	D	19	G
3	D	20	U
3	D	21	A
3	D	22	G
3	D	23	C
3	D	24	U
3	D	27	U
3	D	28	C
3	D	30	G
3	D	32	C
3	D	33	U
3	D	34	C
3	D	37	A
3	D	38	A
3	D	39	C
3	D	40	C
3	D	41	C
3	D	42	G
3	D	43	A
3	D	45	G
3	D	46	A
3	D	47	U
3	D	48	C
3	D	49	G
3	D	50	U
3	D	52	G
3	D	53	G
3	D	57	A
3	D	58	A
3	D	59	A
3	D	61	C
3	D	62	C
3	D	66	C

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Mol	Chain	Res	Type
3	D	70	G
3	D	71	C
3	D	72	A
3	D	73	A
3	D	74	C
3	D	75	C
3	D	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	23	C
3	D	40	C
3	D	44	A
3	D	74	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
4	GNP	A	501	-	28,34,34	1.94	5 (17%)	33,54,54	2.56	11 (33%)
5	MET	D	77	3	6,7,8	0.31	0	4,7,9	0.90	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
4	GNP	A	501	-	-	0/12/38/38	0/3/3/3
5	MET	D	77	3	-	0/4/6/8	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GNP	PB-O3A	-5.79	1.51	1.59
4	A	501	GNP	PB-O2B	-3.19	1.47	1.56
4	A	501	GNP	C8-N7	-2.08	1.30	1.34
4	A	501	GNP	C6-N1	3.43	1.39	1.33
4	A	501	GNP	PG-O1G	5.05	1.51	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GNP	C5-C6-N1	-8.43	112.07	123.59
4	A	501	GNP	C4'-O4'-C1'	-5.12	104.09	109.72
4	A	501	GNP	O3G-PG-O1G	-3.76	103.48	113.49
4	A	501	GNP	PA-O3A-PB	-3.04	122.47	132.67
4	A	501	GNP	C2'-C1'-N9	-2.33	110.73	114.29
4	A	501	GNP	N3-C2-N1	-2.29	123.96	127.44
4	A	501	GNP	O4'-C1'-N9	2.14	112.59	108.10
4	A	501	GNP	C4-C5-N7	2.36	111.65	109.48
4	A	501	GNP	O3G-PG-O2G	2.69	115.54	107.58
4	A	501	GNP	O2B-PB-O1B	3.71	117.75	110.00
4	A	501	GNP	C6-N1-C2	6.29	124.67	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GNP	6	0
5	D	77	MET	5	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	415/415 (100%)	-0.68	9 (2%) 65 50	42, 109, 331, 545	0
2	B	89/89 (100%)	-0.58	3 (3%) 49 34	41, 111, 284, 545	0
3	D	77/77 (100%)	-0.52	0 100 100	64, 113, 208, 345	0
All	All	581/581 (100%)	-0.64	12 (2%) 67 52	41, 110, 284, 545	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.9
1	A	319	ALA	3.8
2	B	183	ILE	3.5
1	A	182	PRO	2.8
1	A	274	THR	2.8
2	B	188	ASN	2.7
1	A	2	ALA	2.7
2	B	248	SER	2.5
1	A	409	GLY	2.4
1	A	397	ILE	2.0
1	A	140	GLY	2.0
1	A	203	LYS	2.0

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(\AA^2)	Q<0.9
5	MET	D	77	8/9	0.91	0.14	-0.41	30,37,111,127	0
4	GNP	A	501	32/32	0.94	0.10	-0.49	28,70,108,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.