



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:29 AM UTC

PDB ID : 1YTU / pdb_00001ytu
Title : Structural basis for 5'-end-specific recognition of the guide RNA strand by the A. fulgidus PIWI protein
Authors : Ma, J.B.; Yuan, Y.R.; Meister, G.; Pei, Y.; Tuschl, T.; Patel, D.J.
Deposited on : 2005-02-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

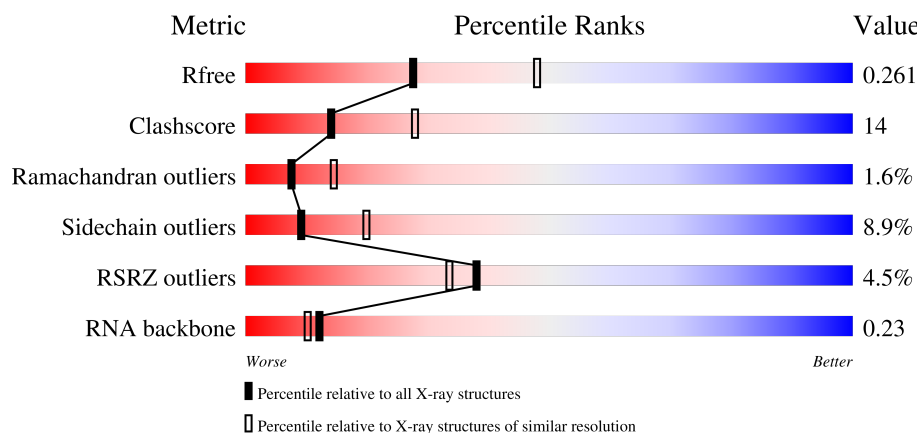
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	6	17% 50% 33% 17%
1	E	6	33% 83% 17%
2	D	4	50% 50% 25% 25%
2	F	4	25% 25% 50% 25%

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Mol	Chain	Length	Quality of chain
3	A	427	3% 62% 28% 5%
3	B	427	4% 69% 24% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7282 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 5'-R(P*AP*GP*AP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	5	Total	C	N	O	P	0	0	0
			110	49	23	33	5			
1	E	6	Total	C	N	O	P	0	0	0
			133	59	28	40	6			

- Molecule 2 is a RNA chain called 5'-R(P*UP*GP*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			83	37	12	30	4			
2	F	4	Total	C	N	O	P	0	0	0
			83	37	12	30	4			

- Molecule 3 is a protein called hypothetical protein AF1318.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	410	Total	C	N	O	S	Se	0	0	0
			3336	2158	550	618	1	9			
3	B	427	Total	C	N	O	S	Se	0	0	0
			3478	2246	579	641	1	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O28951
A	2	MSE	MET	modified residue	UNP O28951
A	112	MSE	MET	modified residue	UNP O28951
A	139	MSE	MET	modified residue	UNP O28951
A	200	MSE	MET	modified residue	UNP O28951
A	208	MSE	MET	modified residue	UNP O28951
A	260	MSE	MET	modified residue	UNP O28951
A	280	MSE	MET	modified residue	UNP O28951

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Chain	Residue	Modelled	Actual	Comment	Reference
A	301	MSE	MET	modified residue	UNP O28951
A	339	MSE	MET	modified residue	UNP O28951
A	377	MSE	MET	modified residue	UNP O28951
B	1	MSE	MET	modified residue	UNP O28951
B	2	MSE	MET	modified residue	UNP O28951
B	112	MSE	MET	modified residue	UNP O28951
B	139	MSE	MET	modified residue	UNP O28951
B	200	MSE	MET	modified residue	UNP O28951
B	208	MSE	MET	modified residue	UNP O28951
B	260	MSE	MET	modified residue	UNP O28951
B	280	MSE	MET	modified residue	UNP O28951
B	301	MSE	MET	modified residue	UNP O28951
B	339	MSE	MET	modified residue	UNP O28951
B	377	MSE	MET	modified residue	UNP O28951

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

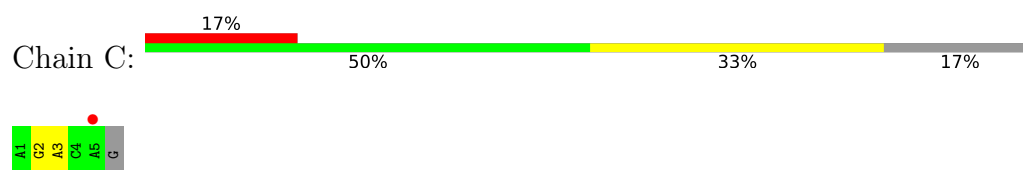
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	3	Total O 3 3	0	0
5	F	1	Total O 1 1	0	0
5	A	21	Total O 21 21	0	0
5	B	30	Total O 30 30	0	0

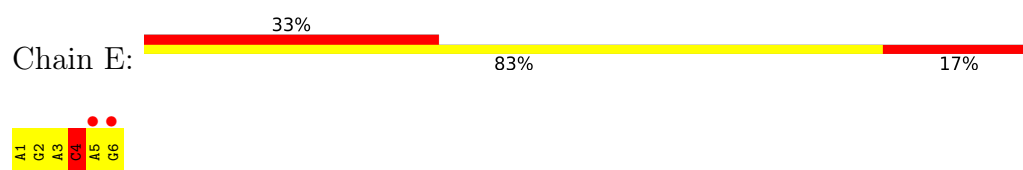
3 Residue-property plots [i](#)

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.

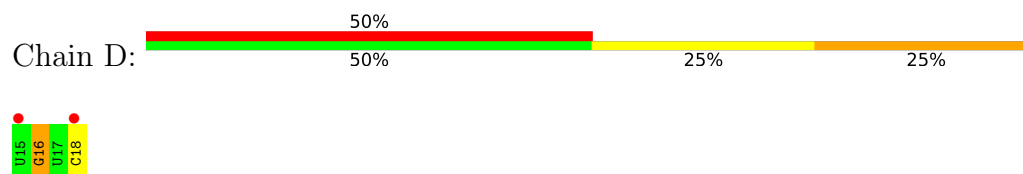
- Molecule 1: 5'-R(P*AP*GP*AP*CP*AP*G)-3'



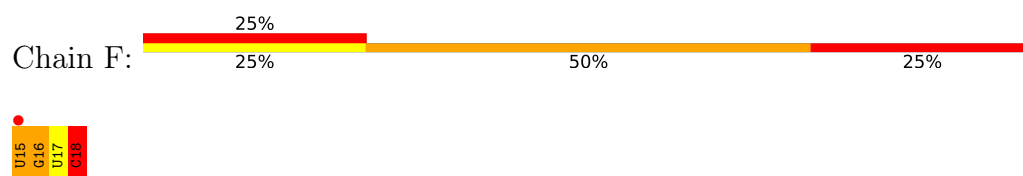
- Molecule 1: 5'-R(P*AP*GP*AP*CP*AP*G)-3'



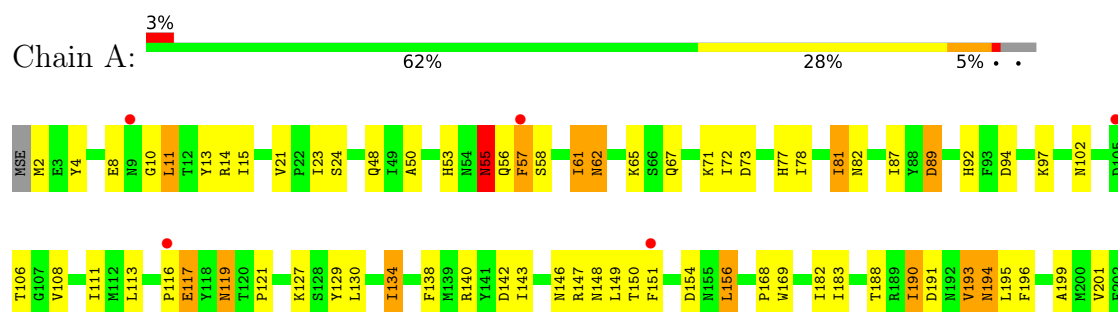
- Molecule 2: 5'-R(P*UP*GP*UP*C)-3'

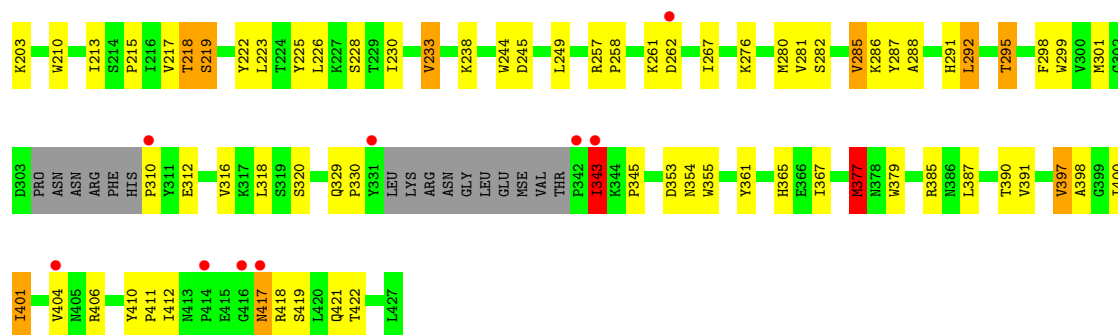


- Molecule 2: 5'-R(P*UP*GP*UP*C)-3'

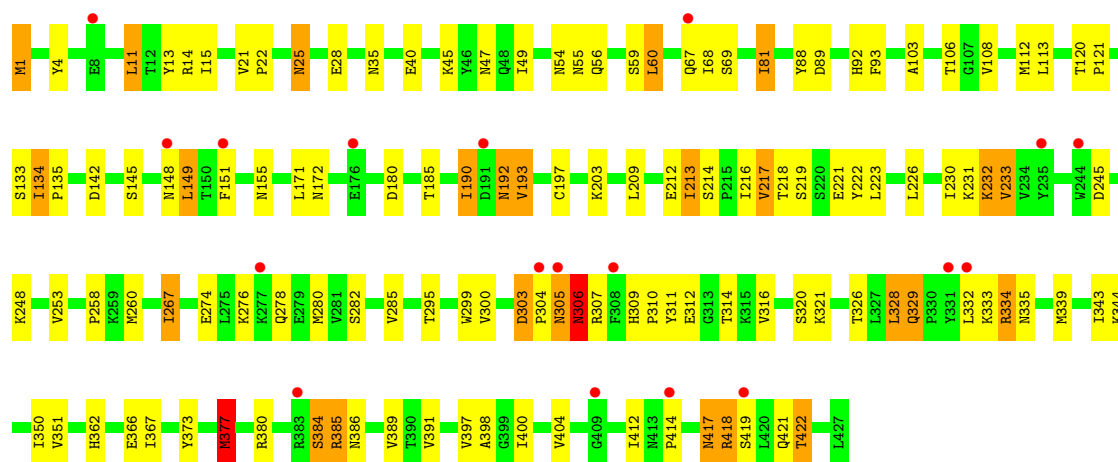


- Molecule 3: hypothetical protein AF1318





• Molecule 3: hypothetical protein AF1318



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	238.75Å 238.75Å 52.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.50) 99.2 (50.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.266 0.203 , 0.261	Depositor DCC
R_{free} test set	1904 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	C	0.80	0/123	1.36	0/188
1	E	0.85	0/149	1.59	4/229 (1.7%)
2	D	0.96	0/91	1.32	0/139
2	F	1.06	1/91 (1.1%)	1.51	1/139 (0.7%)
3	A	0.91	0/3411	1.12	16/4612 (0.3%)
3	B	1.05	3/3556 (0.1%)	1.16	12/4808 (0.2%)
All	All	0.98	4/7421 (0.1%)	1.16	33/10115 (0.3%)

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
3	A	0	1
3	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	339	MSE	SE-CE	6.17	2.13	1.95
3	B	280	MSE	SE-CE	5.87	2.13	1.95
3	B	377	MSE	SE-CE	-5.72	1.78	1.95
2	F	18	C	Cl'-N1	5.72	1.56	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	11	LEU	N-CA-C	7.98	122.11	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	U	C4'-C3'-C2'	-7.92	94.68	102.60
3	B	306	ASN	N-CA-C	-7.85	103.59	113.01
3	A	55	ASN	N-CA-C	7.47	119.77	109.54
1	E	4	C	C4'-C3'-O3'	-7.32	102.02	113.00
3	A	343	ILE	N-CA-C	6.72	118.51	108.23
3	A	343	ILE	CB-CA-C	-6.70	102.86	110.96
3	B	417	ASN	N-CA-C	6.39	118.90	108.55
3	B	303	ASP	CA-C-N	6.23	126.25	119.90
3	B	303	ASP	C-N-CA	6.23	126.25	119.90
3	B	391	VAL	CB-CA-C	-6.17	104.45	111.55
1	E	4	C	O4'-C1'-C2'	-6.15	101.45	107.60
3	B	180	ASP	N-CA-C	-6.12	104.69	111.36
3	A	261	LYS	N-CA-C	6.08	117.78	111.03
3	A	193	VAL	N-CA-C	-6.06	106.83	112.83
3	B	148	ASN	N-CA-C	5.81	119.13	112.97
1	E	3	A	C2'-C3'-O3'	-5.71	105.13	113.70
3	A	156	LEU	N-CA-C	-5.50	105.28	111.28
3	A	226	LEU	N-CA-C	-5.50	105.20	111.14
3	B	385	ARG	N-CA-C	-5.43	102.26	110.24
3	A	73	ASP	N-CA-C	5.38	116.95	111.14
3	A	391	VAL	N-CA-C	-5.37	107.55	111.90
3	B	56	GLN	N-CA-C	5.34	118.58	111.75
3	A	57	PHE	N-CA-C	-5.29	99.53	110.80
3	A	62	ASN	N-CA-C	5.26	118.17	111.69
3	A	194	ASN	N-CA-C	5.23	117.49	109.07
3	B	35	ASN	N-CA-C	5.19	116.62	111.07
3	A	377	MSE	N-CA-C	5.12	119.08	111.87
3	A	285	VAL	N-CA-C	5.09	115.97	109.30
1	E	4	C	N1-C1'-C2'	5.08	119.61	112.00
3	B	398	ALA	N-CA-C	5.08	116.81	111.28
3	B	190	ILE	CB-CA-C	-5.05	105.31	112.14
3	A	353	ASP	N-CA-C	5.04	115.19	108.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	55	ASN	Peptide
3	B	306	ASN	Peptide

5.2 Too-close contacts ⓘ

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	C	110	0	56	1	0
1	E	133	0	67	6	0
2	D	83	0	43	3	0
2	F	83	0	43	6	0
3	A	3336	0	3346	109	0
3	B	3478	0	3494	91	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	21	0	0	4	0
5	B	30	0	0	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
All	All	7282	0	7049	204	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 14.

All (204) 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)
3:B:222:TYR:HD1	3:B:260:MSE:HE2	1.00	1.12
3:B:222:TYR:CD1	3:B:260:MSE:HE2	1.88	1.07
3:A:11:LEU:HD11	5:A:436:HOH:O	1.53	1.05
3:B:305:ASN:HA	3:B:307:ARG:HG3	1.37	1.01
3:A:301:MSE:HE1	3:B:314:THR:HG21	1.53	0.90
3:A:199:ALA:HB1	3:A:233:VAL:HG21	1.56	0.88
3:B:25:ASN:ND2	3:B:28:GLU:H	1.75	0.84
3:A:330:PRO:HB3	3:A:343:ILE:HD11	1.60	0.84
1:E:4:C:H6	1:E:4:C:H5''	1.44	0.83
3:A:199:ALA:CB	3:A:233:VAL:HG21	2.16	0.76
3:B:11:LEU:H	3:B:11:LEU:HD23	1.50	0.76
3:B:418:ARG:O	3:B:422:THR:HB	1.86	0.76
3:B:231:LYS:NZ	3:B:274:GLU:OE1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:ILE:HG22	3:A:24:SER:N	2.02	0.74
3:B:1:MSE:HE2	3:B:1:MSE:O	1.87	0.74
3:A:238:LYS:HE3	3:A:280:MSE:O	1.88	0.73
3:B:377:MSE:O	3:B:389:VAL:HG13	1.89	0.72
3:B:25:ASN:HD22	3:B:28:GLU:H	1.36	0.72
3:A:13:TYR:CE1	3:A:377:MSE:HE1	2.25	0.72
3:B:49:ILE:HD12	3:B:81:ILE:HG21	1.72	0.72
3:A:196:PHE:HZ	3:A:398:ALA:HA	1.54	0.71
3:B:303:ASP:OD2	3:B:306:ASN:HB2	1.91	0.71
3:B:203:LYS:HG3	3:B:209:LEU:HD11	1.73	0.70
3:B:222:TYR:HD1	3:B:260:MSE:CE	1.93	0.70
3:B:54:ASN:HB2	3:B:88:TYR:CZ	2.26	0.70
3:B:300:VAL:HG11	3:B:343:ILE:HD11	1.75	0.69
3:A:276:LYS:HE3	3:A:285:VAL:HG12	1.73	0.69
1:E:4:C:H5''	1:E:4:C:C6	2.28	0.69
3:B:328:LEU:HD23	3:B:386:ASN:HD22	1.58	0.67
3:B:120:THR:HB	3:B:121:PRO:HD3	1.75	0.67
3:A:196:PHE:CZ	3:A:398:ALA:HA	2.29	0.67
3:A:377:MSE:HA	3:A:377:MSE:CE	2.26	0.66
3:B:226:LEU:HD23	3:B:267:ILE:HD11	1.76	0.66
3:B:217:VAL:CG1	3:B:221:GLU:OE1	2.44	0.65
3:B:1:MSE:HE3	3:B:4:TYR:CE1	2.31	0.65
3:A:312:GLU:HB2	3:A:329:GLN:HG3	1.79	0.65
3:B:192:ASN:O	3:B:193:VAL:HG23	1.97	0.64
3:A:285:VAL:O	3:A:354:ASN:ND2	2.31	0.64
3:A:111:ILE:HD12	3:A:134:ILE:HD11	1.79	0.63
3:A:299:TRP:HZ2	3:B:1:MSE:HG2	1.63	0.63
3:B:134:ILE:HG12	3:B:135:PRO:HD2	1.78	0.63
3:B:217:VAL:HG11	3:B:221:GLU:OE1	1.99	0.63
3:B:417:ASN:ND2	3:B:419:SER:H	1.98	0.62
3:A:71:LYS:NZ	3:A:154:ASP:OD1	2.33	0.62
3:B:384:SER:O	3:B:385:ARG:C	2.39	0.61
3:B:217:VAL:HG12	3:B:218:THR:H	1.66	0.61
3:A:14:ARG:HD3	5:A:446:HOH:O	2.01	0.59
3:A:169:TRP:HD1	3:A:377:MSE:HE1	1.66	0.59
3:A:53:HIS:CD2	3:A:61:ILE:HG12	2.37	0.59
3:A:199:ALA:CB	3:A:233:VAL:CG2	2.80	0.59
3:B:54:ASN:HB2	3:B:88:TYR:CE1	2.37	0.59
3:A:11:LEU:HD21	5:A:436:HOH:O	2.03	0.59
2:F:15:U:H2'	2:F:15:U:O2	2.02	0.58
3:B:377:MSE:HE2	3:B:377:MSE:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:102:ASN:O	3:A:106:THR:HG23	2.03	0.58
3:A:23:ILE:CG2	3:A:24:SER:N	2.67	0.57
3:A:299:TRP:CZ2	3:B:1:MSE:HG2	2.38	0.57
3:B:412:ILE:O	3:B:414:PRO:HD3	2.04	0.57
3:B:222:TYR:CD1	3:B:260:MSE:CE	2.75	0.57
3:A:377:MSE:HG3	3:A:377:MSE:O	2.04	0.57
3:A:53:HIS:O	3:A:87:ILE:HA	2.06	0.56
3:B:332:LEU:HG	3:B:333:LYS:N	2.20	0.56
3:A:13:TYR:CE1	3:A:377:MSE:CE	2.88	0.56
3:A:199:ALA:HB3	3:A:233:VAL:CG2	2.36	0.56
3:A:400:ILE:O	3:A:404:VAL:HG23	2.07	0.55
3:B:417:ASN:HD22	3:B:419:SER:H	1.52	0.55
3:A:2:MSE:HE3	3:A:318:LEU:CD2	2.36	0.55
3:A:169:TRP:CD1	3:A:377:MSE:HE1	2.41	0.55
3:A:330:PRO:HB3	3:A:343:ILE:CD1	2.35	0.55
3:A:23:ILE:HG22	3:A:24:SER:H	1.70	0.55
3:B:384:SER:O	3:B:386:ASN:OD1	2.24	0.55
2:D:18:C:H2'	3:A:151:PHE:CD1	2.41	0.55
3:B:414:PRO:O	3:B:421:GLN:HG3	2.07	0.55
3:A:53:HIS:CD2	3:A:55:ASN:H	2.25	0.55
3:B:321:LYS:HD2	3:B:350:ILE:O	2.08	0.54
2:F:17:U:O2'	3:B:334:ARG:NH2	2.40	0.54
3:A:143:ILE:O	3:A:147:ARG:HG2	2.08	0.54
3:B:14:ARG:HD3	3:B:172:ASN:OD1	2.07	0.54
3:B:11:LEU:HD23	3:B:11:LEU:N	2.22	0.53
3:B:151:PHE:O	3:B:155:ASN:ND2	2.35	0.53
3:A:140:ARG:NH2	3:A:142:ASP:OD2	2.42	0.53
3:A:119:ASN:OD1	3:A:121:PRO:HD2	2.09	0.53
2:D:18:C:H2'	3:A:151:PHE:CE1	2.44	0.52
3:B:295:THR:O	3:B:344:LYS:HE3	2.09	0.52
1:E:1:A:H61	3:B:120:THR:HA	1.74	0.52
2:D:16:G:H2'	2:D:16:G:N3	2.23	0.52
3:A:213:ILE:HD13	3:A:401:ILE:HD11	1.91	0.52
3:A:377:MSE:HA	3:A:377:MSE:HE3	1.92	0.52
3:B:362:HIS:NE2	3:B:366:GLU:OE2	2.43	0.52
3:B:377:MSE:O	3:B:389:VAL:CG1	2.57	0.51
3:A:230:ILE:O	3:A:233:VAL:HG23	2.11	0.51
2:F:16:G:H2'	2:F:17:U:H6	1.75	0.51
3:A:244:TRP:C	3:A:244:TRP:CD1	2.89	0.51
3:B:185:THR:O	3:B:253:VAL:HA	2.11	0.51
3:B:230:ILE:O	3:B:233:VAL:HG12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:299:TRP:C	3:A:299:TRP:CD1	2.89	0.50
3:A:417:ASN:ND2	3:A:419:SER:OG	2.44	0.50
3:B:171:LEU:HD21	3:B:377:MSE:HE3	1.94	0.50
3:B:1:MSE:HE3	3:B:4:TYR:HE1	1.72	0.50
3:B:305:ASN:CA	3:B:307:ARG:HG3	2.25	0.50
3:B:332:LEU:HG	3:B:333:LYS:H	1.77	0.50
3:B:400:ILE:O	3:B:404:VAL:HG23	2.12	0.50
3:A:288:ALA:HB2	3:A:355:TRP:CZ2	2.47	0.50
3:A:130:LEU:HD22	3:A:134:ILE:HD11	1.94	0.49
3:A:23:ILE:CG2	3:A:24:SER:H	2.25	0.49
3:A:287:TYR:CD1	3:A:287:TYR:C	2.90	0.49
3:A:301:MSE:HE3	3:B:4:TYR:CE2	2.47	0.49
2:F:17:U:O2'	2:F:18:C:H5'	2.13	0.49
3:A:48:GLN:NE2	3:A:82:ASN:HB2	2.28	0.49
3:A:299:TRP:NE1	3:A:301:MSE:HG2	2.28	0.49
3:A:330:PRO:CB	3:A:343:ILE:HD11	2.39	0.48
3:A:249:LEU:O	3:A:287:TYR:HA	2.13	0.48
3:B:231:LYS:HE2	3:B:278:GLN:HE22	1.78	0.48
3:A:195:LEU:HD11	3:A:222:TYR:HB2	1.96	0.48
3:A:13:TYR:HE1	3:A:377:MSE:CE	2.27	0.47
3:A:298:PHE:HB2	3:A:345:PRO:HG3	1.95	0.47
3:A:422:THR:O	3:A:422:THR:CG2	2.62	0.47
3:A:169:TRP:CD1	3:A:377:MSE:CE	2.97	0.47
3:B:21:VAL:HG13	3:B:22:PRO:HD2	1.96	0.47
3:B:223:LEU:HD21	3:B:260:MSE:HE3	1.95	0.47
3:A:223:LEU:HB3	3:A:267:ILE:HD12	1.96	0.47
3:A:286:LYS:NZ	5:A:429:HOH:O	2.44	0.47
3:B:1:MSE:HB3	3:B:316:VAL:CG1	2.45	0.47
3:B:40:GLU:HA	5:B:434:HOH:O	2.13	0.47
3:A:127:LYS:HZ1	3:A:400:ILE:HD11	1.80	0.47
3:A:199:ALA:HB3	3:A:233:VAL:HG22	1.95	0.47
3:B:11:LEU:HD13	3:B:373:TYR:CD2	2.49	0.46
3:B:49:ILE:CD1	3:B:81:ILE:HG21	2.44	0.46
3:A:182:ILE:HG21	3:A:390:THR:HG21	1.96	0.46
3:A:78:ILE:CG2	3:A:81:ILE:HD11	2.46	0.46
3:A:195:LEU:HD21	3:A:258:PRO:HD3	1.96	0.46
3:A:77:HIS:CD2	3:A:77:HIS:N	2.83	0.46
3:A:4:TYR:HE2	3:B:304:PRO:HG3	1.81	0.46
3:A:196:PHE:HZ	3:A:398:ALA:CA	2.26	0.46
3:B:213:ILE:HD11	3:B:397:VAL:HG11	1.97	0.46
3:A:50:ALA:HB2	3:A:108:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:190:ILE:HD11	3:B:216:ILE:HG12	1.97	0.46
3:A:111:ILE:HD12	3:A:134:ILE:CD1	2.45	0.46
3:A:210:TRP:HA	3:A:421:GLN:O	2.16	0.46
3:A:217:VAL:CG1	3:A:218:THR:N	2.78	0.46
3:A:301:MSE:HE3	3:B:4:TYR:CD2	2.50	0.46
3:A:67:GLN:HE22	3:A:150:THR:HA	1.80	0.46
3:A:116:PRO:HB2	3:A:117:GLU:HG3	1.97	0.45
3:A:410:TYR:CD1	3:A:410:TYR:N	2.83	0.45
1:E:1:A:N6	3:B:120:THR:HA	2.31	0.45
3:B:222:TYR:HB3	3:B:260:MSE:HE1	1.98	0.45
3:A:257:ARG:HB2	3:A:258:PRO:HD2	1.98	0.45
3:A:182:ILE:CG2	3:A:390:THR:HG21	2.47	0.45
3:A:195:LEU:CD1	3:A:222:TYR:HB2	2.47	0.45
3:B:60:LEU:HD11	3:B:145:SER:HA	1.99	0.45
2:F:16:G:O2'	2:F:17:U:H5'	2.17	0.44
3:A:385:ARG:C	3:A:387:LEU:H	2.24	0.44
3:B:223:LEU:CD2	3:B:260:MSE:HE3	2.47	0.44
3:B:258:PRO:HB2	3:B:260:MSE:HG3	1.99	0.44
3:A:61:ILE:O	3:A:65:LYS:HB2	2.17	0.44
3:A:203:LYS:HG3	3:A:244:TRP:HH2	1.82	0.44
3:B:103:ALA:O	3:B:106:THR:HB	2.17	0.44
1:E:4:C:H2'	1:E:5:A:O4'	2.17	0.44
3:A:67:GLN:NE2	3:A:150:THR:HA	2.32	0.43
3:A:48:GLN:HE22	3:A:82:ASN:HB2	1.84	0.43
3:A:295:THR:HB	3:B:299:TRP:HE1	1.83	0.43
1:C:2:G:H2'	1:C:3:A:O4'	2.19	0.43
3:A:361:TYR:CE1	3:A:365:HIS:HE1	2.36	0.43
3:A:10:GLY:O	3:A:11:LEU:HG	2.19	0.43
3:B:68:ILE:HD13	3:B:112:MSE:SE	2.68	0.43
3:B:312:GLU:O	3:B:326:THR:O	2.37	0.43
2:F:15:U:N3	2:F:16:G:C8	2.87	0.43
3:A:418:ARG:HA	3:A:421:GLN:OE1	2.19	0.43
3:A:291:HIS:C	3:A:292:LEU:HD23	2.44	0.43
3:B:92:HIS:O	3:B:93:PHE:C	2.62	0.43
3:B:197:CYS:HB2	3:B:214:SER:HB3	2.00	0.43
3:A:190:ILE:HG22	3:A:191:ASP:N	2.33	0.43
3:A:225:TYR:HA	3:A:228:SER:HB3	2.01	0.43
3:A:97:LYS:HE3	3:A:129:TYR:CZ	2.55	0.42
3:B:212:GLU:HG3	3:B:232:LYS:HB3	2.01	0.42
3:B:134:ILE:HG12	3:B:135:PRO:CD	2.45	0.42
3:B:171:LEU:CD2	3:B:377:MSE:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:397:VAL:O	3:A:398:ALA:C	2.62	0.42
3:B:1:MSE:HE3	3:B:4:TYR:OH	2.20	0.42
3:B:309:HIS:O	3:B:311:TYR:N	2.52	0.42
3:B:192:ASN:O	3:B:193:VAL:CB	2.67	0.42
3:A:215:PRO:HB2	3:A:217:VAL:HG23	2.02	0.42
3:B:13:TYR:HE2	3:B:377:MSE:CE	2.32	0.42
3:B:311:TYR:HD2	3:B:329:GLN:HE21	1.68	0.42
3:A:130:LEU:HD12	3:A:138:PHE:CZ	2.55	0.42
3:A:195:LEU:HG	3:A:219:SER:HA	2.01	0.42
3:B:1:MSE:HE3	3:B:4:TYR:CZ	2.54	0.42
3:B:377:MSE:HE3	3:B:377:MSE:HB2	1.90	0.42
3:A:2:MSE:HE3	3:A:318:LEU:HD21	2.02	0.41
3:A:183:ILE:HG12	3:A:201:VAL:HG22	2.02	0.41
3:A:361:TYR:CE1	3:A:365:HIS:CE1	3.08	0.41
3:B:303:ASP:OD2	3:B:306:ASN:CB	2.66	0.41
3:A:2:MSE:HE2	3:A:316:VAL:HG11	2.02	0.41
3:B:192:ASN:O	3:B:193:VAL:CG2	2.65	0.41
1:E:1:A:O2'	1:E:2:G:OP1	2.36	0.41
3:A:410:TYR:HA	3:A:411:PRO:HD2	1.94	0.41
3:A:377:MSE:HA	3:A:377:MSE:HE2	2.00	0.41
3:B:245:ASP:OD1	3:B:282:SER:HB2	2.21	0.41
3:B:276:LYS:HE2	3:B:285:VAL:HG12	2.03	0.41
3:A:245:ASP:OD1	3:A:282:SER:HB2	2.21	0.40
3:A:148:ASN:O	3:A:149:LEU:C	2.64	0.40
3:A:191:ASP:H	3:A:194:ASN:HB2	1.87	0.40
3:A:168:PRO:HD2	3:A:379:TRP:CE2	2.57	0.40
3:A:310:PRO:HG2	3:A:343:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	404/427 (95%)	375 (93%)	23 (6%)	6 (2%)	8	16
3	B	425/427 (100%)	396 (93%)	22 (5%)	7 (2%)	7	14
All	All	829/854 (97%)	771 (93%)	45 (5%)	13 (2%)	7	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	193	VAL
3	B	219	SER
3	B	305	ASN
3	B	384	SER
3	A	57	PHE
3	A	89	ASP
3	A	56	GLN
3	A	119	ASN
3	B	149	LEU
3	A	397	VAL
3	B	310	PRO
3	B	15	ILE
3	A	15	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	
3	A	378/383 (99%)	345 (91%)	33 (9%)	9	21
3	B	394/383 (103%)	358 (91%)	36 (9%)	9	19
All	All	772/766 (101%)	703 (91%)	69 (9%)	9	20

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	8	GLU
3	A	21	VAL
3	A	58	SER

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Mol	Chain	Res	Type
3	A	61	ILE
3	A	62	ASN
3	A	72	ILE
3	A	81	ILE
3	A	89	ASP
3	A	92	HIS
3	A	94	ASP
3	A	113	LEU
3	A	117	GLU
3	A	134	ILE
3	A	146	ASN
3	A	156	LEU
3	A	188	THR
3	A	190	ILE
3	A	193	VAL
3	A	218	THR
3	A	219	SER
3	A	233	VAL
3	A	262	ASP
3	A	281	VAL
3	A	292	LEU
3	A	295	THR
3	A	320	SER
3	A	343	ILE
3	A	367	ILE
3	A	377	MSE
3	A	401	ILE
3	A	406	ARG
3	A	412	ILE
3	A	417	ASN
3	B	1	MSE
3	B	11	LEU
3	B	25	ASN
3	B	45	LYS
3	B	47	ASN
3	B	55	ASN
3	B	59	SER
3	B	60	LEU
3	B	67	GLN
3	B	69	SER
3	B	81	ILE
3	B	89	ASP

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Mol	Chain	Res	Type
3	B	108	VAL
3	B	113	LEU
3	B	133	SER
3	B	134	ILE
3	B	142	ASP
3	B	149	LEU
3	B	192	ASN
3	B	213	ILE
3	B	217	VAL
3	B	232	LYS
3	B	233	VAL
3	B	248	LYS
3	B	267	ILE
3	B	320	SER
3	B	328	LEU
3	B	329	GLN
3	B	334	ARG
3	B	335	ASN
3	B	351	VAL
3	B	367	ILE
3	B	377	MSE
3	B	380	ARG
3	B	418	ARG
3	B	422	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	48	GLN
3	A	53	HIS
3	A	67	GLN
3	A	148	ASN
3	A	211	ASN
3	A	291	HIS
3	A	365	HIS
3	A	417	ASN
3	B	25	ASN
3	B	47	ASN
3	B	56	GLN
3	B	92	HIS
3	B	102	ASN
3	B	278	GLN

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Mol	Chain	Res	Type
3	B	306	ASN
3	B	309	HIS
3	B	417	ASN
3	B	423	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	4/6 (66%)	0	0
1	E	5/6 (83%)	2 (40%)	0
2	D	3/4 (75%)	1 (33%)	0
2	F	3/4 (75%)	2 (66%)	0
All	All	15/20 (75%)	5 (33%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	16	G
1	E	4	C
1	E	6	G
2	F	16	G
2	F	18	C

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	C	5/6 (83%)	0.63	1 (20%) 3 2	46, 61, 70, 73	1 (20%)
1	E	6/6 (100%)	1.40	2 (33%) 1 1	50, 52, 61, 79	2 (33%)
2	D	4/4 (100%)	2.11	2 (50%) 0 0	54, 100, 102, 103	1 (25%)
2	F	4/4 (100%)	2.12	1 (25%) 2 1	51, 99, 102, 102	1 (25%)
3	A	401/427 (93%)	0.32	14 (3%) 47 42	40, 60, 82, 97	0
3	B	416/427 (97%)	0.50	18 (4%) 40 35	43, 56, 82, 95	0
All	All	836/874 (95%)	0.44	38 (4%) 38 33	40, 58, 82, 103	5 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	148	ASN	5.0
1	E	6	G	4.6
2	F	15	U	4.4
1	C	5	A	4.3
1	E	5	A	4.3
3	B	414	PRO	3.7
2	D	15	U	3.7
3	B	331	TYR	3.4
3	B	191	ASP	3.4
3	B	332	LEU	3.3
3	B	151	PHE	3.2
3	A	116	PRO	3.0
3	B	383	ARG	2.8
3	A	414	PRO	2.7
3	A	151	PHE	2.6
3	B	176	GLU	2.6
3	B	244	TRP	2.5
3	A	57	PHE	2.5
3	B	67	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	305	ASN	2.5
3	A	262	ASP	2.5
3	A	416	GLY	2.4
3	B	8	GLU	2.4
3	B	409	GLY	2.4
3	B	419	SER	2.4
3	A	343	ILE	2.4
3	A	417	ASN	2.4
3	B	235	TYR	2.3
3	A	9	ASN	2.3
3	B	308	PHE	2.3
3	A	404	VAL	2.3
3	A	342	PRO	2.3
3	B	277	LYS	2.3
3	B	304	PRO	2.2
3	A	310	PRO	2.1
2	D	18	C	2.1
3	A	105	ASP	2.1
3	A	331	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	MG	A	428	1/1	0.99	0.09	48,48,48,48	0
4	MG	B	428	1/1	0.99	0.11	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.