



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:53 PM GMT

PDB ID : 1YTU
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
<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

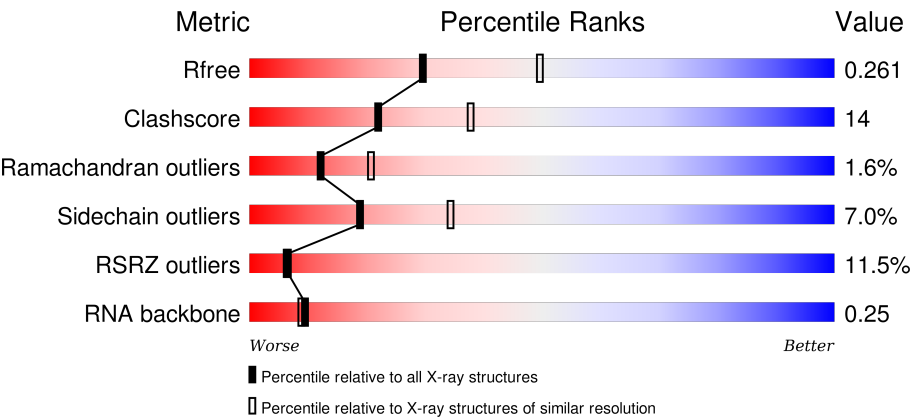
1 Overall quality at a glance i

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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	C	6	<div><div>17%</div><div>33%33%17%17%</div></div>
1	E	6	<div><div>33%</div><div>17%17%50%17%</div></div>
2	D	4	<div><div>100%</div><div>25%50%25%</div></div>
2	F	4	<div><div>25%</div><div>75%25%</div></div>

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Mol	Chain	Length	Quality of chain
3	A	427	<div><div></div><div>12%</div><div>66%</div><div>26%</div><div></div><div></div></div>
3	B	427	<div><div></div><div>9%</div><div>72%</div><div>24%</div><div></div><div></div></div>

2 Entry composition

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 (three-letter code: MG) (formula: Mg).

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

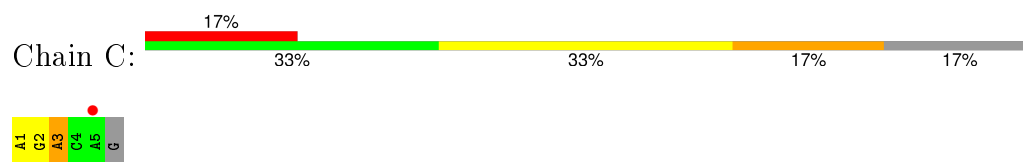
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0
5	B	30	Total O 30 30	0	0
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

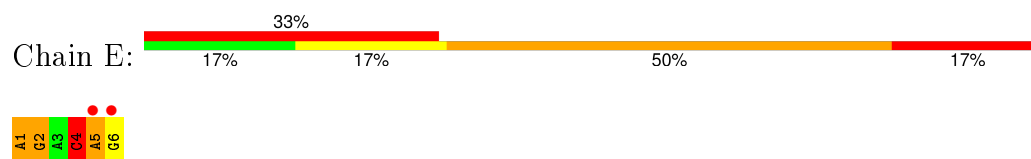
3 Residue-property plots [i](#)

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.

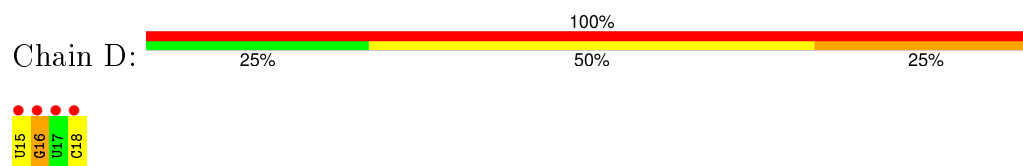
- Molecule 1: 5'-R(P*AP*GP*AP*CP*AP*G)-3'



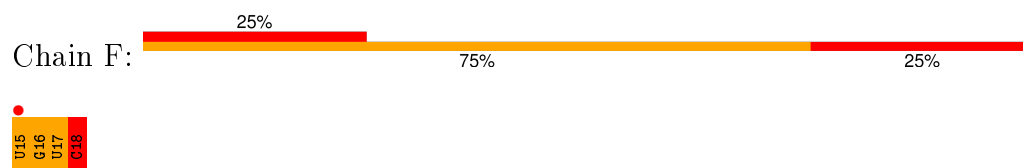
- Molecule 1: 5'-R(P*AP*GP*AP*CP*AP*G)-3'



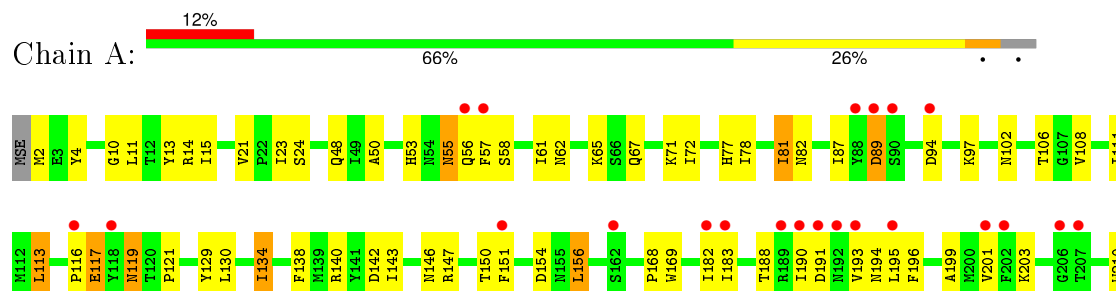
- Molecule 2: 5'-R(P*UP*GP*UP*C)-3'

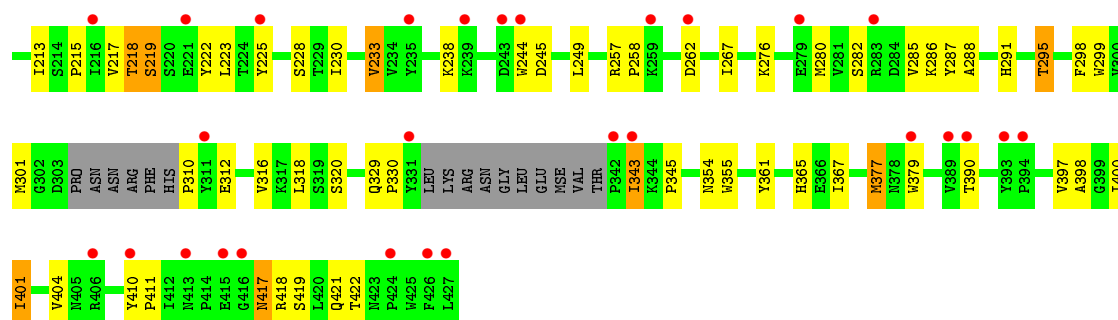


- Molecule 2: 5'-R(P*UP*GP*UP*C)-3'

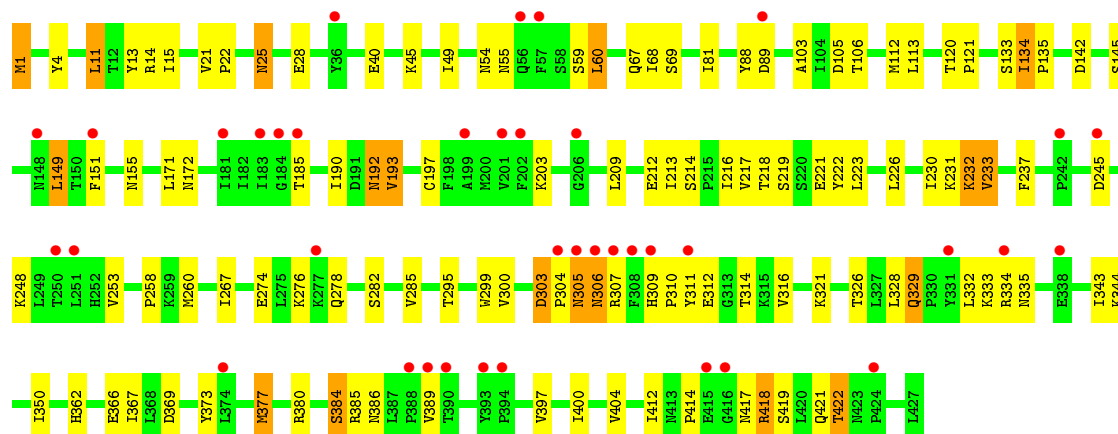


- Molecule 3: hypothetical protein AF1318





- 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 34.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.50) 99.2 (34.46-2.50)	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 (5.28%)	DCC
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 , 58.8	EDS
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37959 reflections	Xtriage
F_o, F_c correlation	0.95	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, 0.375 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: 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	1.53	1/123 (0.8%)	1.90	2/188 (1.1%)
1	E	1.51	1/149 (0.7%)	1.95	6/229 (2.6%)
2	D	1.15	0/91	1.72	1/139 (0.7%)
2	F	1.29	0/91	2.05	4/139 (2.9%)
3	A	0.75	0/3411	0.81	2/4612 (0.0%)
3	B	0.86	0/3556	0.87	2/4808 (0.0%)
All	All	0.86	2/7421 (0.0%)	0.95	17/10115 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	A	OP3-P	-10.10	1.49	1.61
1	C	1	A	OP3-P	-9.55	1.49	1.61

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	C	O5'-P-OP1	-8.12	98.39	105.70
2	F	15	U	C4'-C3'-C2'	-7.92	94.68	102.60
3	B	369	ASP	CB-CG-OD1	6.95	124.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	U	O4'-C1'-N1	6.42	113.33	108.20
1	E	4	C	C6-N1-C2	-6.39	117.75	120.30
1	E	5	A	O4'-C1'-N9	6.24	113.19	108.20
1	E	2	G	C5-C6-O6	-5.94	125.04	128.60
1	E	1	A	N1-C2-N3	-5.67	126.46	129.30
1	C	1	A	C1'-O4'-C4'	-5.50	105.50	109.90
1	E	4	C	C5-C6-N1	5.47	123.74	121.00
3	A	156	LEU	CB-CG-CD2	-5.41	101.81	111.00
2	F	18	C	C6-N1-C2	-5.36	118.16	120.30
2	F	17	U	O4'-C1'-N1	5.32	112.46	108.20
1	C	3	A	N1-C2-N3	-5.23	126.69	129.30
3	A	113	LEU	CA-CB-CG	5.22	127.30	115.30
3	B	105	ASP	CB-CG-OD1	-5.05	113.76	118.30
2	D	15	U	C3'-C2'-C1'	-5.01	97.49	101.50

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	104	0
3	B	3478	0	3494	90	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	198	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 (198) 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:418:ARG:O	3:B:422:THR:HB	1.86	0.76
3:B:11:LEU:H	3:B:11:LEU:HD23	1.50	0.76
3:B:231:LYS:NZ	3:B:274:GLU:OE1	2.19	0.75
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:B:49:ILE:HD12	3:B:81:ILE:HG21	1.72	0.72
3:A:13:TYR:CE1	3:A:377:MSE:HE1	2.25	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:C6	1:E:4:C:H5''	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:PHE:CZ	3:A:398:ALA:HA	2.29	0.67
3:A:377:MSE:CE	3:A:377:MSE:HA	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:217:VAL:HG12	3:B:218:THR:H	1.66	0.61
3:A:169:TRP:HD1	3:A:377:MSE:HE1	1.66	0.59
3:A:14:ARG:HD3	5:A:446:HOH:O	2.01	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
3:B:377:MSE:HA	3:B:377:MSE:HE2	1.85	0.58
2:F:15:U:H2'	2:F:15:U:O2	2.02	0.58
3:A:102:ASN:O	3:A:106:THR:HG23	2.03	0.58
3:A:377:MSE:HG3	3:A:377:MSE:O	2.04	0.58
3:A:299:TRP:CZ2	3:B:1:MSE:HG2	2.38	0.57
3:A:23:ILE:CG2	3:A:24:SER:N	2.67	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: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:199:ALA:HB3	3:A:233:VAL:CG2	2.36	0.56
3:A:13:TYR:CE1	3:A:377:MSE:CE	2.88	0.56
3:B:384:SER:O	3:B:385:ARG:C	2.39	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:330:PRO:HB3	3:A:343:ILE:CD1	2.35	0.55
3:A:169:TRP:CD1	3:A:377:MSE:HE1	2.41	0.55
3:A:2:MSE:HE3	3:A:318:LEU:CD2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	3:B:11:LEU:HD23	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:377:MSE:HA	3:A:377:MSE:HE3	1.92	0.52
3:A:213:ILE:HD13	3:A:401:ILE:HD11	1.91	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: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
3:B:171:LEU:HD21	3:B:377:MSE:HE3	1.94	0.50
3:A:417:ASN:ND2	3:A:419:SER:OG	2.44	0.50
3:B:305:ASN:CA	3:B:307:ARG:HG3	2.25	0.50
3:B:1:MSE:HE3	3:B:4:TYR:HE1	1.72	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:301:MSE:HE3	3:B:4:TYR:CE2	2.47	0.49
3:A:299:TRP:NE1	3:A:301:MSE:HG2	2.28	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:330:PRO:CB	3:A:343:ILE:HD11	2.39	0.48
3:B:231:LYS:HE2	3:B:278:GLN:HE22	1.78	0.48
3:A:249:LEU:O	3:A:287:TYR:HA	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:298:PHE:HB2	3:A:345:PRO:HG3	1.95	0.47
3:A:422:THR:CG2	3:A:422:THR:O	2.62	0.47
3:A:169:TRP:CD1	3:A:377:MSE:CE	2.97	0.47
3:B:223:LEU:HD21	3:B:260:MSE:HE3	1.95	0.47
3:B:21:VAL:HG13	3:B:22:PRO:HD2	1.96	0.47
3:A:223:LEU:HB3	3:A:267:ILE:HD12	1.96	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: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:195:LEU:HD21	3:A:258:PRO:HD3	1.96	0.46
3:A:78:ILE:CG2	3:A:81:ILE:HD11	2.46	0.46
3:A:77:HIS:CD2	3:A:77:HIS:N	2.83	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:4:TYR:HE2	3:B:304:PRO:HG3	1.81	0.46
3:A:244:TRP:CD1	3:A:244:TRP:C	2.89	0.46
3:A:50:ALA:HB2	3:A:108:VAL:HG11	1.97	0.46
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:299:TRP:C	3:A:299:TRP:CD1	2.89	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:410:TYR:N	3:A:410:TYR:CD1	2.83	0.45
3:A:116:PRO:HB2	3:A:117:GLU:HG3	1.97	0.45
3:B:222:TYR:HB3	3:B:260:MSE:HE1	1.98	0.45
1:E:1:A:N6	3:B:120:THR:HA	2.31	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:A:287:TYR:CD1	3:A:287:TYR:C	2.90	0.45
3:B:60:LEU:HD11	3:B:145:SER:HA	1.99	0.45
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
2:F:16:G:O2'	2:F:17:U:H5'	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:312:GLU:O	3:B:326:THR:O	2.37	0.43
3:B:68:ILE:HD13	3:B:112:MSE:SE	2.68	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:B:197:CYS:HB2	3:B:214:SER:HB3	2.00	0.43
3:A:225:TYR:HA	3:A:228:SER:HB3	2.01	0.43
3:A:190:ILE:HG22	3:A:191:ASP:N	2.33	0.43
3:B:212:GLU:HG3	3:B:232:LYS:HB3	2.01	0.42
3:A:97:LYS:HE3	3:A:129:TYR:CZ	2.55	0.42
3:B:171:LEU:CD2	3:B:377:MSE:HE3	2.49	0.42
3:B:134:ILE:HG12	3:B:135:PRO:CD	2.45	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:A:286:LYS:NZ	5:A:429:HOH:O	2.44	0.42
3:B:192:ASN:O	3:B:193:VAL:CB	2.67	0.42
3:B:13:TYR:HE2	3:B:377:MSE:CE	2.32	0.42
3:A:215:PRO:HB2	3:A:217:VAL:HG23	2.02	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:361:TYR:CE1	3:A:365:HIS:CE1	3.08	0.41
3:A:183:ILE:HG12	3:A:201:VAL:HG22	2.02	0.41
3:B:303:ASP:OD2	3:B:306:ASN:CB	2.66	0.41
3:B:192:ASN:O	3:B:193:VAL:CG2	2.65	0.41
3:A:2:MSE:HE2	3:A:316:VAL:HG11	2.02	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:HE2	3:A:377:MSE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:ASP:OD1	3:A:282:SER:HB2	2.21	0.40
3:A:191:ASP:H	3:A:194:ASN:HB2	1.87	0.40
3:A:310:PRO:HG2	3:A:343:ILE:HD11	2.03	0.40
3:A:168:PRO:HD2	3:A:379:TRP:CE2	2.57	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%)	13	22
3	B	425/427 (100%)	396 (93%)	22 (5%)	7 (2%)	12	21
All	All	829/854 (97%)	771 (93%)	45 (5%)	13 (2%)	12	21

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%)	352 (93%)	26 (7%)	19	35
3	B	394/383 (103%)	366 (93%)	28 (7%)	18	34
All	All	772/766 (101%)	718 (93%)	54 (7%)	19	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	21	VAL
3	A	58	SER
3	A	62	ASN
3	A	72	ILE
3	A	81	ILE
3	A	89	ASP
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	193	VAL
3	A	218	THR
3	A	219	SER
3	A	233	VAL
3	A	262	ASP
3	A	291	HIS
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	417	ASN
3	B	1	MSE

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Mol	Chain	Res	Type
3	B	11	LEU
3	B	25	ASN
3	B	45	LYS
3	B	55	ASN
3	B	59	SER
3	B	60	LEU
3	B	67	GLN
3	B	69	SER
3	B	89	ASP
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	232	LYS
3	B	233	VAL
3	B	237	PHE
3	B	248	LYS
3	B	303	ASP
3	B	329	GLN
3	B	335	ASN
3	B	367	ILE
3	B	377	MSE
3	B	380	ARG
3	B	418	ARG
3	B	422	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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	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

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Mol	Chain	Res	Type
3	B	278	GLN
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 carbohydrates 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%)	0.51	1 (20%) 1 1	61, 62, 73, 77	1 (20%)
1	E	6/6 (100%)	1.11	2 (33%) 0 0	51, 61, 84, 90	2 (33%)
2	D	4/4 (100%)	2.84	4 (100%) 0 0	97, 100, 102, 103	1 (25%)
2	F	4/4 (100%)	1.21	1 (25%) 1 1	93, 99, 102, 102	1 (25%)
3	A	401/427 (93%)	0.54	50 (12%) 5 5	40, 60, 82, 97	0
3	B	416/427 (97%)	0.47	38 (9%) 11 12	43, 56, 82, 95	0
All	All	836/874 (95%)	0.53	96 (11%) 6 6	40, 58, 83, 103	5 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	305	ASN	7.2
3	A	283	ARG	5.4
3	A	57	PHE	5.3
1	E	6	G	5.2
3	B	308	PHE	4.5
3	B	148	ASN	4.4
3	B	56	GLN	4.3
2	D	15	U	4.1
1	C	5	A	4.1
3	A	190	ILE	3.9
3	B	416	GLY	3.8
3	B	331	TYR	3.7
3	B	307	ARG	3.7
3	B	277	LYS	3.6
3	A	244	TRP	3.6
3	B	304	PRO	3.6
3	A	243	ASP	3.5
3	A	89	ASP	3.4
3	A	191	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	379	TRP	3.4
3	A	151	PHE	3.4
3	B	184	GLY	3.4
3	A	413	ASN	3.4
3	A	259	LYS	3.3
3	B	334	ARG	3.3
3	A	331	TYR	3.3
3	B	151	PHE	3.3
3	B	183	ILE	3.2
3	A	195	LEU	3.2
3	B	245	ASP	3.2
3	A	189	ARG	3.1
3	A	193	VAL	3.1
3	A	415	GLU	3.1
3	A	416	GLY	3.0
3	A	393	TYR	3.0
3	B	389	VAL	3.0
3	A	342	PRO	3.0
3	A	207	THR	2.9
3	A	90	SER	2.9
3	B	388	PRO	2.9
3	B	57	PHE	2.8
3	A	390	THR	2.8
3	A	201	VAL	2.8
3	A	424	PRO	2.8
3	A	192	ASN	2.7
2	D	16	G	2.7
3	A	406	ARG	2.7
3	A	389	VAL	2.7
3	A	225	TYR	2.7
3	B	309	HIS	2.6
3	B	390	THR	2.6
3	A	94	ASP	2.6
1	E	5	A	2.5
3	A	202	PHE	2.5
3	A	279	GLU	2.5
3	A	116	PRO	2.5
3	B	202	PHE	2.5
3	B	374	LEU	2.4
3	A	311	TYR	2.4
3	A	221	GLU	2.4
3	A	183	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	206	GLY	2.4
3	A	427	LEU	2.4
3	A	426	PHE	2.4
3	B	311	TYR	2.3
3	B	251	LEU	2.3
3	B	185	THR	2.3
3	B	199	ALA	2.3
3	A	88	TYR	2.3
3	B	394	PRO	2.3
3	B	201	VAL	2.3
3	A	162	SER	2.3
3	B	415	GLU	2.3
2	D	17	U	2.2
2	D	18	C	2.2
3	A	182	ILE	2.2
3	A	118	TYR	2.2
3	A	235	TYR	2.2
3	A	239	LYS	2.2
2	F	15	U	2.2
3	A	56	GLN	2.2
3	A	262	ASP	2.2
3	B	393	TYR	2.2
3	B	181	ILE	2.1
3	B	306	ASN	2.1
3	B	250	THR	2.1
3	A	216	ILE	2.1
3	A	343	ILE	2.1
3	B	424	PRO	2.1
3	A	394	PRO	2.1
3	B	206	GLY	2.1
3	B	89	ASP	2.1
3	B	338	GLU	2.0
3	A	410	TYR	2.0
3	B	36	TYR	2.0
3	B	242	PRO	2.0

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

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
4	MG	B	428	1/1	0.97	0.03	-2.76	31,31,31,31	0
4	MG	A	428	1/1	0.95	0.04	-2.82	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.