Full wwPDB X-ray Structure Validation Report (i)

May 27, 2024 – 09:28 PM EDT

PDB ID	:	6MFR
Title	:	Human Argonaute2-miR-122 bound to a target RNA with three central mismatches (bu3)
Authors	:	Sheu-Gruttadauria, J.; MacRae, I.J.
Deposited on	:	2018-09-12
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

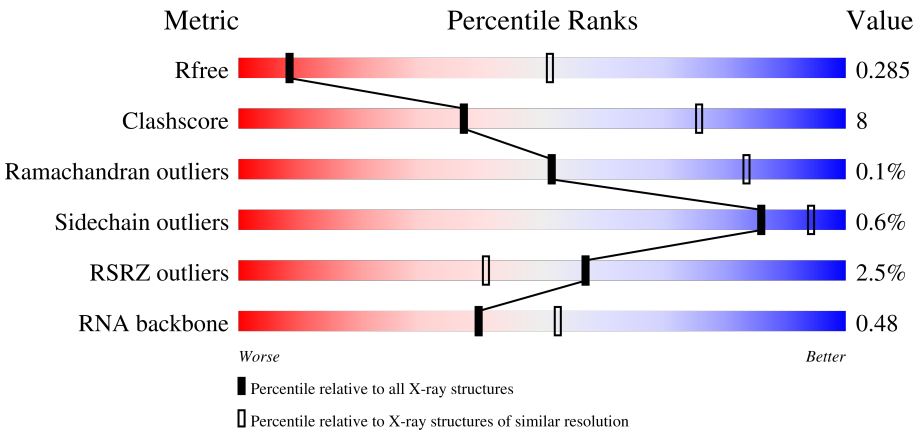
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	859	.% 76% 17% 7%
1	B	859	2% 76% 16% 7%
2	C	21	14% 29% 48% 14% 5% 5%
2	D	21	19% 19% 29% 19% 33%

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Mol	Chain	Length	Quality of chain
3	E	23	13% 48% 39% 9%
3	F	23	9% 48% 13% 30%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14309 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	802	6431	4095	1156	1139	41	0	0	0
1	B	795	6366	4056	1141	1129	40	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8
A	669	ALA	ASP	engineered mutation	UNP Q9UKV8
A	824	ALA	SER	engineered mutation	UNP Q9UKV8
A	828	ASP	SER	engineered mutation	UNP Q9UKV8
A	831	ASP	SER	engineered mutation	UNP Q9UKV8
A	834	ALA	SER	engineered mutation	UNP Q9UKV8
B	387	ASP	SER	engineered mutation	UNP Q9UKV8
B	669	ALA	ASP	engineered mutation	UNP Q9UKV8
B	824	ALA	SER	engineered mutation	UNP Q9UKV8
B	828	ASP	SER	engineered mutation	UNP Q9UKV8
B	831	ASP	SER	engineered mutation	UNP Q9UKV8
B	834	ALA	SER	engineered mutation	UNP Q9UKV8

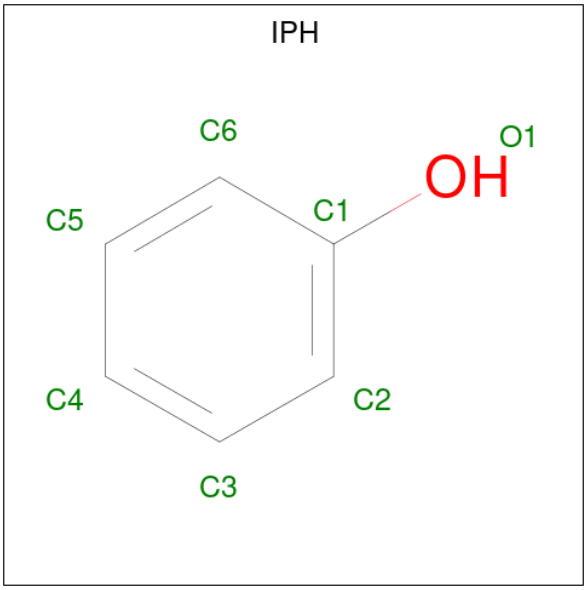
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*GP*GP*AP*GP*UP*GP*UP*GP*AP*CP*AP*AP*UP*GP*GP*UP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	20	433	192	77	144	20	0	0	0
2	D	14	308	136	58	100	14	0	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*AP*AP*CP*AP*CP*CP*AP*UP*UP*UP*UP*CP*AP*CP*AP*CP*UP*CP*CP*AP*AP*A)-3').

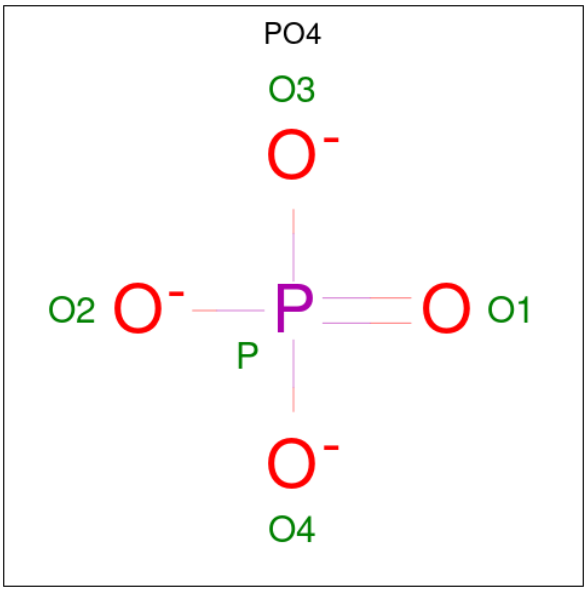
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	22	443	198	77	146	22	0	0	0
			Total	C	N	O	P			
3	F	16	295	131	50	99	15	0	0	1

- Molecule 4 is PHENOL (three-letter code: IPH) (formula: C_6H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	6	1	0	0
			Total	C	O		
4	A	1	7	6	1	0	0
			Total	C	O		
4	B	1	7	6	1	0	0
			Total	C	O		
4	B	1	7	6	1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



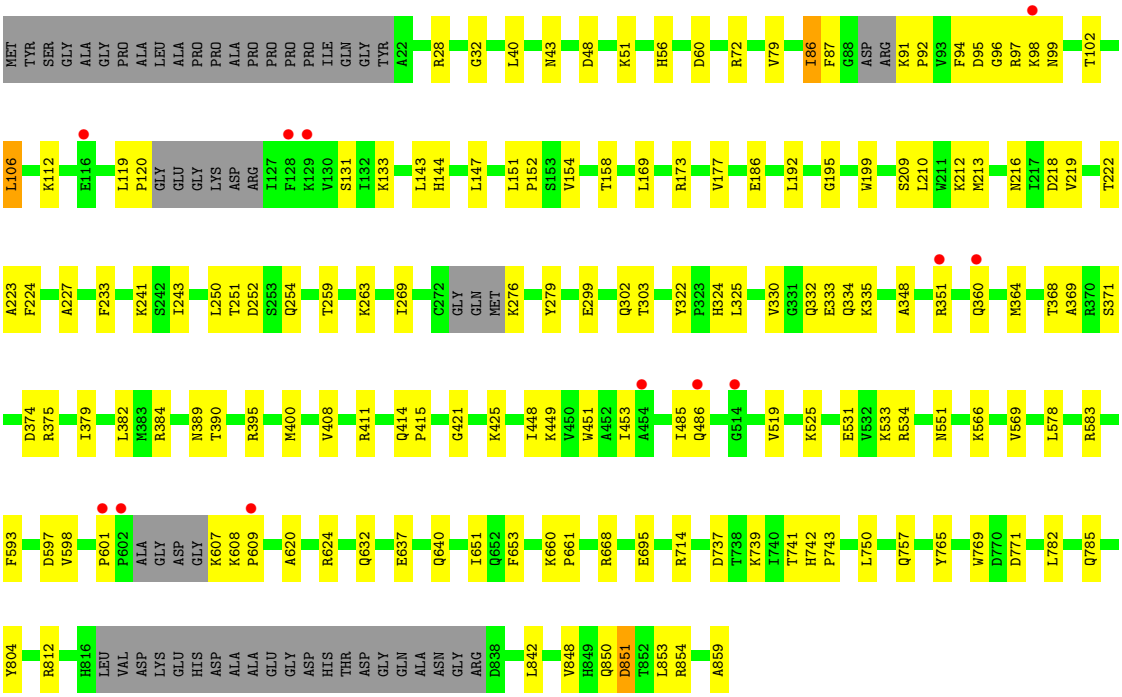
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	B	1	5	4	1	0	0

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.

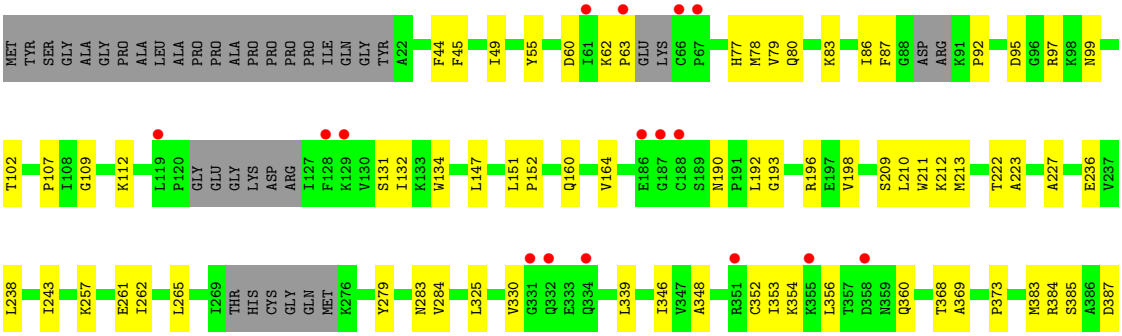
• Molecule 1: Protein argonaute-2

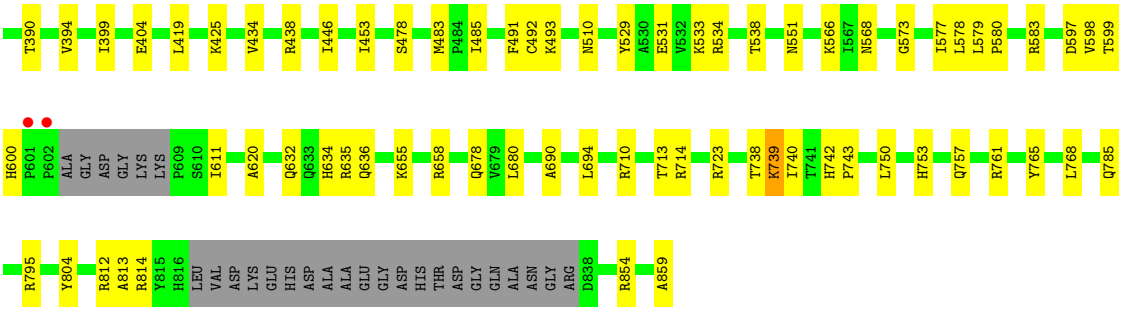
Chain A:



• Molecule 1: Protein argonaute-2

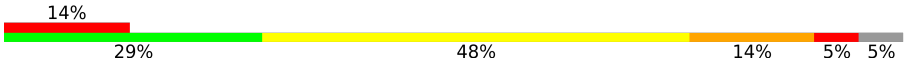
Chain B:

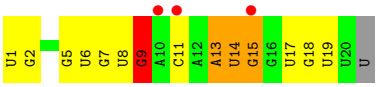




• Molecule 2: RNA (5'-R(P*UP*GP*GP*AP*GP*UP*GP*UP*GP*AP*CP*AP*AP*UP*GP*GP*UP*GP*UP*U)-3')

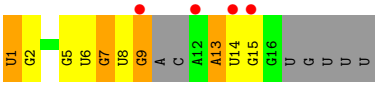
Chain C:





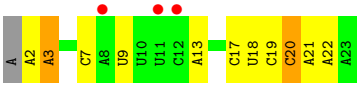
• Molecule 2: RNA (5'-R(P*UP*GP*GP*AP*GP*UP*GP*UP*GP*AP*CP*AP*AP*UP*GP*GP*UP*GP*UP*U)-3')

Chain D:



• Molecule 3: RNA (5'-R(P*AP*AP*AP*CP*AP*CP*CP*AP*UP*UP*UP*UP*CP*AP*CP*AP*CP*UP*CP*CP*AP*AP*A)-3')

Chain E:



• Molecule 3: RNA (5'-R(P*AP*AP*AP*CP*AP*CP*CP*AP*UP*UP*UP*UP*CP*AP*CP*AP*CP*UP*CP*CP*AP*AP*A)-3')

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.17Å 137.96Å 153.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.42 – 3.60 39.42 – 3.57	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.42-3.60) 98.3 (39.42-3.57)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.239 , 0.283 0.243 , 0.285	Depositor DCC
R_{free} test set	1386 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	84.8	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	14309	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3803e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IPH, PO4

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	0.25	0/6583	0.47	0/8909
1	B	0.24	0/6516	0.47	0/8820
2	C	0.61	1/484 (0.2%)	1.17	3/752 (0.4%)
2	D	0.65	1/344 (0.3%)	0.92	0/532
3	E	0.35	0/492	1.02	0/761
3	F	0.23	0/325	0.80	1/499 (0.2%)
All	All	0.28	2/14744 (0.0%)	0.56	4/20273 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-10.52	1.48	1.61
2	D	1	U	OP3-P	-10.52	1.48	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	9	G	C8-N9-C4	-12.92	101.23	106.40
2	C	9	G	N7-C8-N9	9.06	117.63	113.10
2	C	9	G	C5'-C4'-O4'	-7.97	99.54	109.10
3	F	11	U	P-O3'-C3'	5.32	126.09	119.70

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	6431	0	6493	102	1
1	B	6366	0	6418	93	1
2	C	433	0	214	12	0
2	D	308	0	152	13	0
3	E	443	0	228	12	0
3	F	295	0	154	7	0
4	A	14	0	12	1	0
4	B	14	0	12	1	0
5	B	5	0	0	0	0
All	All	14309	0	13683	215	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (215) 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:566:LYS:NZ	1:B:859:ALA:OXT	2.02	0.93
1:A:97:ARG:HD3	3:E:7:C:H5"	1.57	0.87
1:B:761:ARG:NH1	2:D:9:G:O6	2.07	0.85
2:C:9:G:H21	3:E:13:A:H61	1.26	0.82
1:B:192:LEU:HB2	1:B:196:ARG:HB2	1.64	0.80
1:A:60:ASP:HB3	1:A:131:SER:HB2	1.66	0.77
1:A:351:ARG:NH2	2:C:9:G:OP1	2.19	0.76
1:A:147:LEU:HD11	1:A:213:MET:HG2	1.68	0.75
1:B:531:GLU:OE2	1:B:534:ARG:NH1	2.20	0.73
1:B:97:ARG:NE	3:F:7:C:OP1	2.22	0.72
1:A:241:LYS:O	1:B:510:ASN:ND2	2.22	0.72
1:A:95:ASP:HB2	1:A:99:ASN:HB3	1.72	0.72
1:A:583:ARG:NH1	1:A:620:ALA:O	2.23	0.71
1:A:651:ILE:HA	4:A:901:IPH:H4	1.76	0.67
2:C:14:U:H4'	2:C:15:G:OP1	1.93	0.67
1:A:186:GLU:OE1	1:B:854:ARG:NH2	2.27	0.67
1:A:209:SER:OG	1:A:739:LYS:O	2.08	0.67
3:E:19:C:H2'	3:E:20:C:H5'	1.76	0.66
1:B:600:HIS:O	3:F:12:C:O2'	2.14	0.65
1:B:551:ASN:ND2	2:D:2:G:OP2	2.29	0.64
1:A:227:ALA:HB2	1:A:348:ALA:HB2	1.80	0.64
1:B:632:GLN:NE2	1:B:636:GLN:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:OE1	1:B:655:LYS:NZ	2.29	0.63
2:C:9:G:O5'	2:C:9:G:C8	2.52	0.63
1:A:660:LYS:NZ	1:A:695:GLU:OE1	2.25	0.62
2:C:9:G:N2	3:E:13:A:H61	1.97	0.62
1:A:389:ASN:O	1:A:395:ARG:NH2	2.34	0.61
1:B:227:ALA:HB2	1:B:348:ALA:HB2	1.83	0.60
1:B:583:ARG:NH1	1:B:620:ALA:O	2.34	0.60
1:B:680:LEU:HD22	1:B:768:LEU:HB3	1.83	0.60
1:B:261:GLU:HA	1:B:354:LYS:NZ	2.16	0.60
1:B:95:ASP:OD1	1:B:99:ASN:HB2	2.01	0.59
1:B:529:TYR:HE2	2:D:1:U:OP2	1.85	0.59
1:A:757:GLN:OE1	2:C:5:G:N2	2.36	0.58
1:B:599:THR:CG2	1:B:814:ARG:HH11	2.17	0.58
1:B:599:THR:HG21	1:B:814:ARG:HD2	1.85	0.58
1:B:60:ASP:HB3	1:B:131:SER:HB2	1.86	0.57
1:B:446:ILE:HD11	1:B:573:GLY:HA3	1.86	0.57
1:A:28:ARG:NH2	1:A:742:HIS:O	2.38	0.57
1:A:112:LYS:HG2	1:A:133:LYS:HE2	1.88	0.56
1:A:578:LEU:HD13	1:A:785:GLN:HG2	1.88	0.56
1:B:261:GLU:O	1:B:354:LYS:NZ	2.39	0.56
1:A:48:ASP:HB3	1:A:400:MET:HB2	1.88	0.55
1:A:449:LYS:HG3	1:A:486:GLN:HG3	1.88	0.55
1:A:714:ARG:NH2	2:C:7:G:OP2	2.39	0.55
1:A:210:LEU:HD23	1:A:743:PRO:HA	1.88	0.55
1:A:566:LYS:NZ	1:A:566:LYS:HB3	2.22	0.55
2:C:6:U:HO2'	2:C:7:G:H8	1.55	0.55
1:B:678:GLN:OE1	1:B:678:GLN:N	2.39	0.54
3:E:2:A:O2'	3:E:3:A:O5'	2.25	0.54
1:A:209:SER:OG	1:A:210:LEU:N	2.40	0.54
3:E:19:C:C2'	3:E:20:C:H5'	2.36	0.54
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.89	0.54
1:B:261:GLU:HA	1:B:354:LYS:HZ3	1.72	0.54
1:A:453:ILE:HD13	1:A:519:VAL:HB	1.90	0.54
1:B:86:ILE:HG22	1:B:87:PHE:H	1.72	0.53
1:B:190:ASN:HB2	1:B:198:VAL:HB	1.89	0.53
1:A:224:PHE:CZ	1:A:351:ARG:HG2	2.43	0.53
1:B:45:PHE:CE2	1:B:383:MET:HG2	2.44	0.53
1:B:80:GLN:HA	1:B:83:LYS:HE3	1.90	0.53
1:B:196:ARG:NH2	1:B:354:LYS:HB2	2.23	0.53
1:B:209:SER:OG	1:B:739:LYS:O	2.21	0.53
3:E:18:U:H2'	3:E:19:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD13	1:B:785:GLN:HG2	1.90	0.53
1:A:276:LYS:NZ	1:A:276:LYS:HB3	2.24	0.53
1:B:534:ARG:O	1:B:538:THR:OG1	2.23	0.53
1:B:757:GLN:OE1	2:D:5:G:N2	2.41	0.53
1:A:371:SER:OG	1:A:374:ASP:OD1	2.26	0.52
1:B:92:PRO:HB3	1:B:102:THR:HG22	1.91	0.52
1:B:151:LEU:HD12	1:B:152:PRO:HD2	1.91	0.52
3:F:6:C:H2'	3:F:7:C:C6	2.43	0.52
1:A:209:SER:HB3	1:A:212:LYS:O	2.09	0.52
1:B:86:ILE:HG23	1:B:107:PRO:HD2	1.92	0.52
1:A:632:GLN:OE1	1:A:640:GLN:N	2.27	0.52
1:A:637:GLU:O	1:A:668:ARG:NH2	2.43	0.52
1:B:49:ILE:HD12	1:B:213:MET:HG3	1.91	0.52
1:A:151:LEU:HD12	1:A:152:PRO:HD2	1.91	0.52
1:B:753:HIS:NE2	2:D:6:U:OP1	2.42	0.52
1:A:86:ILE:HG22	1:A:87:PHE:H	1.75	0.51
1:A:551:ASN:ND2	2:C:2:G:OP2	2.41	0.51
1:A:750:LEU:HB3	1:A:765:TYR:HE1	1.75	0.51
1:A:769:TRP:NE1	1:A:771:ASP:OD1	2.43	0.51
1:B:262:ILE:HD12	1:B:265:LEU:HD12	1.91	0.51
1:B:238:LEU:HD23	1:B:257:LYS:HD3	1.92	0.51
1:A:384:ARG:NH1	1:B:658:ARG:HD3	2.27	0.50
1:A:601:PRO:HG3	1:A:608:LYS:O	2.12	0.50
1:B:192:LEU:O	1:B:360:GLN:HG2	2.10	0.50
1:A:250:LEU:H	1:A:254:GLN:HE22	1.58	0.50
1:A:421:GLY:HA2	1:A:425:LYS:HA	1.92	0.50
3:F:11:U:H1'	3:F:12:C:OP2	2.12	0.50
1:A:32:GLY:HA3	1:A:411:ARG:NH2	2.27	0.49
1:A:243:ILE:HD11	1:A:325:LEU:HD21	1.92	0.49
1:A:218:ASP:OD1	1:A:375:ARG:NH1	2.46	0.49
1:A:210:LEU:HD12	1:A:739:LYS:H	1.77	0.49
2:C:8:U:O4	2:C:9:G:N2	2.45	0.49
1:B:369:ALA:HB2	2:D:7:G:H4'	1.95	0.49
1:A:119:LEU:HD12	1:A:120:PRO:HD2	1.94	0.48
1:A:199:TRP:HB2	1:A:224:PHE:CD1	2.48	0.48
2:D:13:A:H4'	2:D:13:A:OP1	2.13	0.48
1:A:192:LEU:O	1:A:360:GLN:HG2	2.12	0.48
1:B:78:MET:HE3	1:B:132:ILE:HD11	1.95	0.48
1:B:419:LEU:HD23	1:B:577:ILE:HD11	1.94	0.48
1:B:394:VAL:HG13	1:B:399:ILE:HB	1.95	0.48
1:A:333:GLU:OE2	1:A:333:GLU:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:HG11	1:A:351:ARG:NH1	2.29	0.48
3:E:17:C:H2'	3:E:18:U:C6	2.49	0.47
1:B:210:LEU:HD12	1:B:211:TRP:N	2.30	0.47
1:B:387:ASP:HB3	1:B:390:THR:OG1	2.14	0.47
1:B:714:ARG:NH2	2:D:7:G:OP2	2.48	0.47
1:A:147:LEU:HD21	1:A:213:MET:HE1	1.96	0.47
1:A:222:THR:OG1	1:A:223:ALA:N	2.48	0.47
1:B:279:TYR:HB3	1:B:330:VAL:HB	1.97	0.47
1:B:384:ARG:HH21	1:B:404:GLU:HA	1.79	0.47
1:A:169:LEU:HD11	1:A:173:ARG:CZ	2.44	0.46
1:A:251:THR:OG1	1:A:252:ASP:N	2.48	0.46
1:A:737:ASP:HA	1:A:741:THR:HG21	1.97	0.46
1:B:597:ASP:OD1	1:B:598:VAL:N	2.48	0.46
1:A:742:HIS:CG	1:A:743:PRO:HD2	2.51	0.46
1:A:850:GLN:O	1:A:854:ARG:NH1	2.49	0.46
1:A:369:ALA:HB2	2:C:7:G:H4'	1.97	0.46
3:E:20:C:O2'	3:E:21:A:OP1	2.27	0.46
1:A:302:GLN:HB3	1:A:303:THR:H	1.52	0.46
1:B:750:LEU:HB3	1:B:765:TYR:HE2	1.81	0.46
1:A:609:PRO:HG2	1:A:842:LEU:HD11	1.98	0.46
2:C:13:A:H4'	2:C:14:U:OP1	2.16	0.46
1:A:322:TYR:HB3	1:A:325:LEU:HD13	1.98	0.45
1:A:451:TRP:HZ3	1:A:453:ILE:HD11	1.81	0.45
1:B:279:TYR:HD2	1:B:339:LEU:HD11	1.81	0.45
1:A:566:LYS:HE2	1:A:859:ALA:OXT	2.16	0.45
1:A:143:LEU:HD13	1:A:158:THR:HG21	1.98	0.45
1:B:738:THR:O	1:B:740:ILE:N	2.44	0.45
1:A:653:PHE:CD1	1:A:661:PRO:HG3	2.51	0.45
1:B:44:PHE:HE1	1:B:713:THR:HG23	1.81	0.45
2:D:9:G:H21	3:F:13:A:H62	1.64	0.45
1:B:425:LYS:HE2	1:B:425:LYS:HB3	1.82	0.45
1:B:634:HIS:HD2	1:B:635:ARG:HG3	1.81	0.45
1:B:77:HIS:HA	1:B:80:GLN:HG2	1.98	0.45
1:B:710:ARG:NH2	2:D:9:G:C4	2.84	0.45
2:D:6:U:O2'	2:D:7:G:H5'	2.17	0.45
1:A:279:TYR:HB3	1:A:330:VAL:HG11	1.98	0.45
1:B:79:VAL:O	1:B:83:LYS:HG3	2.17	0.45
1:B:193:GLY:O	1:B:236:GLU:HB3	2.17	0.45
1:B:243:ILE:HD11	1:B:325:LEU:HD11	1.99	0.45
1:B:742:HIS:CG	1:B:743:PRO:HD2	2.52	0.45
1:B:196:ARG:NH1	1:B:356:LEU:HD21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:OG1	1:B:223:ALA:N	2.50	0.44
1:B:694:LEU:HD11	4:B:902:IPH:C1	2.47	0.44
1:A:259:THR:HG22	1:A:263:LYS:HE3	1.98	0.44
1:B:611:ILE:HG21	1:B:813:ALA:HB3	2.00	0.44
1:A:56:HIS:CE1	1:A:99:ASN:ND2	2.86	0.44
1:B:279:TYR:CD2	1:B:339:LEU:HD11	2.53	0.44
1:B:352:CYS:SG	1:B:353:ILE:N	2.90	0.44
1:A:848:VAL:HG23	1:A:853:LEU:HG	1.98	0.44
1:B:209:SER:HB3	1:B:212:LYS:O	2.17	0.44
1:B:533:LYS:HE3	1:B:812:ARG:HH12	1.82	0.44
1:A:97:ARG:NH1	1:A:98:LYS:HD2	2.32	0.44
1:A:98:LYS:O	1:A:98:LYS:CG	2.66	0.44
1:A:250:LEU:HB3	1:A:254:GLN:CD	2.38	0.44
1:A:533:LYS:HD2	1:A:812:ARG:NH1	2.33	0.44
1:B:478:SER:OG	1:B:485:ILE:HG12	2.18	0.44
1:A:91:LYS:HB2	1:A:91:LYS:NZ	2.33	0.43
1:A:566:LYS:HB3	1:A:566:LYS:HZ2	1.82	0.43
1:B:109:GLY:O	1:B:134:TRP:HB3	2.18	0.43
1:B:283:ASN:OD1	1:B:284:VAL:N	2.41	0.43
1:A:414:GLN:HA	1:A:415:PRO:HD3	1.89	0.43
1:A:750:LEU:HB3	1:A:765:TYR:CE1	2.53	0.43
1:A:86:ILE:HG21	1:A:106:LEU:HD13	2.00	0.43
1:A:195:GLY:HA3	1:A:233:PHE:CE2	2.53	0.43
1:A:448:ILE:HB	1:A:485:ILE:HD13	1.99	0.43
1:A:51:LYS:HD3	1:A:144:HIS:CE1	2.53	0.43
1:A:72:ARG:NH2	1:A:95:ASP:O	2.52	0.43
3:F:6:C:H2'	3:F:7:C:H6	1.84	0.43
1:B:750:LEU:HB3	1:B:765:TYR:CE2	2.54	0.43
2:D:9:G:N2	3:F:13:A:H62	2.16	0.43
3:E:20:C:O2'	3:E:21:A:P	2.77	0.43
1:A:98:LYS:O	1:A:98:LYS:HG3	2.18	0.43
1:A:269:ILE:HD12	1:A:279:TYR:HE2	1.84	0.42
1:B:434:VAL:HG13	1:B:795:ARG:HG2	2.01	0.42
1:A:40:LEU:HB2	1:A:408:VAL:HG13	2.01	0.42
1:A:332:GLN:OE1	1:A:334:GLN:NE2	2.49	0.42
1:A:332:GLN:HB2	1:A:335:LYS:HB2	1.99	0.42
1:A:43:ASN:ND2	1:A:216:ASN:OD1	2.53	0.42
1:B:160:GLN:O	1:B:164:VAL:HG23	2.19	0.42
3:E:19:C:N4	3:E:20:C:H41	2.17	0.42
1:B:483:MET:SD	1:B:568:ASN:HB2	2.60	0.42
3:E:19:C:C2	3:E:20:C:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:O	1:A:379:ILE:HG13	2.19	0.42
1:B:55:TYR:HD2	1:B:134:TRP:CZ3	2.38	0.42
1:B:533:LYS:HD2	1:B:812:ARG:NH2	2.35	0.42
1:A:94:PHE:CE2	1:A:96:GLY:HA2	2.55	0.42
1:A:219:VAL:HG12	1:A:382:LEU:HD22	2.01	0.42
2:D:7:G:H2'	2:D:8:U:C6	2.55	0.42
1:A:531:GLU:HG3	1:A:534:ARG:HH11	1.85	0.41
1:B:209:SER:O	1:B:743:PRO:HB3	2.20	0.41
1:A:525:LYS:HA	1:A:525:LYS:HD3	1.89	0.41
1:A:593:PHE:HE1	1:A:782:LEU:HD21	1.84	0.41
1:B:112:LYS:NZ	1:B:112:LYS:HB3	2.35	0.41
1:B:579:LEU:HA	1:B:580:PRO:HD3	1.92	0.41
1:B:147:LEU:HD11	1:B:213:MET:HG2	2.02	0.41
1:B:491:PHE:CE2	1:B:493:LYS:HD3	2.55	0.41
1:B:373:PRO:HG3	1:B:723:ARG:HD3	2.02	0.41
1:A:79:VAL:HA	1:A:87:PHE:CE2	2.55	0.41
1:B:62:LYS:HB3	1:B:63:PRO:HD3	2.03	0.41
1:B:196:ARG:NH1	1:B:356:LEU:CD2	2.84	0.41
1:A:324:HIS:CD2	1:A:325:LEU:HD12	2.55	0.41
1:A:364:MET:O	1:A:368:THR:HG22	2.21	0.41
1:A:851:ASP:N	1:A:851:ASP:OD1	2.54	0.41
1:A:569:VAL:O	1:A:624:ARG:NH2	2.44	0.40
1:A:390:THR:HA	1:A:395:ARG:HH21	1.86	0.40
1:B:453:ILE:O	1:B:492:CYS:HA	2.21	0.40
1:B:690:ALA:O	1:B:694:LEU:HB2	2.21	0.40
1:A:209:SER:O	1:A:743:PRO:HB3	2.22	0.40
1:B:262:ILE:HD11	1:B:346:ILE:HD11	2.04	0.40
1:A:597:ASP:OD1	1:A:598:VAL:N	2.53	0.40
1:B:680:LEU:HB2	1:B:768:LEU:HD13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:OE2	1:B:438:ARG:NH2[4_477]	1.97	0.23

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/859 (92%)	746 (94%)	44 (6%)	0	100	100
1	B	781/859 (91%)	736 (94%)	43 (6%)	2 (0%)	41	75
All	All	1571/1718 (91%)	1482 (94%)	87 (6%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	385	SER
1	B	739	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	711/749 (95%)	705 (99%)	6 (1%)	81	91
1	B	703/749 (94%)	701 (100%)	2 (0%)	92	97
All	All	1414/1498 (94%)	1406 (99%)	8 (1%)	86	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	106	LEU
1	A	154	VAL
1	A	607	LYS

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Mol	Chain	Res	Type
1	A	804	TYR
1	A	851	ASP
1	B	368	THR
1	B	804	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	204	GLN
1	A	254	GLN
1	A	553	GLN
1	B	634	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	19/21 (90%)	6 (31%)	3 (15%)
2	D	12/21 (57%)	5 (41%)	0
3	E	20/23 (86%)	4 (20%)	1 (5%)
3	F	12/23 (52%)	1 (8%)	1 (8%)
All	All	63/88 (71%)	16 (25%)	5 (7%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	11	C
2	C	14	U
2	C	15	G
2	C	17	U
2	C	18	G
2	C	19	U
2	D	7	G
2	D	9	G
2	D	13	A
2	D	14	U
2	D	15	G
3	E	3	A
3	E	9	U
3	E	20	C

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Mol	Chain	Res	Type
3	E	22	A
3	F	12	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	9	G
2	C	13	A
2	C	14	U
3	E	20	C
3	F	11	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	IPH	B	902	-	7,7,7	0.34	0	8,8,8	0.23	0
4	IPH	A	901	-	7,7,7	0.33	0	8,8,8	0.24	0
4	IPH	A	902	-	7,7,7	0.37	0	8,8,8	0.25	0
4	IPH	B	903	-	7,7,7	0.34	0	8,8,8	0.22	0
5	PO4	B	901	-	4,4,4	0.91	0	6,6,6	0.43	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	IPH	A	901	-	-	-	0/1/1/1
4	IPH	B	902	-	-	-	0/1/1/1
4	IPH	B	903	-	-	-	0/1/1/1
4	IPH	A	902	-	-	-	0/1/1/1

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	902	IPH	1	0
4	A	901	IPH	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 (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	802/859 (93%)	0.02	12 (1%)	73	60	30, 91, 155, 240	0
1	B	795/859 (92%)	-0.02	18 (2%)	60	44	33, 89, 161, 227	0
2	C	20/21 (95%)	0.98	3 (15%)	2	1	65, 173, 247, 289	0
2	D	14/21 (66%)	1.18	4 (28%)	0	0	50, 86, 224, 231	0
3	E	22/23 (95%)	1.19	3 (13%)	3	2	88, 169, 223, 249	0
3	F	16/23 (69%)	0.83	2 (12%)	3	2	80, 108, 255, 300	0
All	All	1669/1806 (92%)	0.05	42 (2%)	57	41	30, 91, 170, 300	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	GLY	6.7
1	B	66	CYS	4.8
3	F	12	C	4.8
3	E	12	C	4.6
3	E	8	A	4.1
2	D	9	G	4.0
1	B	186	GLU	3.9
1	A	602	PRO	3.7
1	A	609	PRO	3.5
1	B	334	GLN	3.5
1	A	514	GLY	3.5
1	A	454	ALA	3.3
3	E	11	U	3.3
1	B	63	PRO	3.3
1	B	188	CYS	3.2
1	B	332	GLN	3.2
2	C	11	C	3.2
2	C	15	G	3.0
1	B	67	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	116	GLU	2.9
1	A	129	LYS	2.9
1	A	486	GLN	2.8
3	F	13	A	2.8
1	B	128	PHE	2.8
1	A	128	PHE	2.7
2	D	12	A	2.7
1	A	601	PRO	2.6
2	D	14	U	2.5
1	B	129	LYS	2.4
1	B	358	ASP	2.4
1	B	602	PRO	2.3
1	B	351	ARG	2.3
2	D	15	G	2.2
1	B	119	LEU	2.2
1	A	360	GLN	2.2
1	B	61	ILE	2.1
2	C	10	A	2.1
1	A	98	LYS	2.0
1	B	355	LYS	2.0
1	A	351	ARG	2.0
1	B	601	PRO	2.0
1	B	331	GLY	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	B	901	5/5	0.75	0.21	205,206,209,210	0
4	IPH	B	902	7/7	0.82	0.49	130,130,132,132	0
4	IPH	B	903	7/7	0.89	0.40	93,94,96,98	0
4	IPH	A	902	7/7	0.89	0.47	95,95,97,98	0
4	IPH	A	901	7/7	0.91	0.46	120,121,122,122	0

6.5 Other polymers (i)

There are no such residues in this entry.