W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:12 AM GMT

PDB ID	:	3HKM
Title	:	Crystal Structure of rice(Oryza sativa) Rrp46
Authors	:	Yang, C.-C.; Wang, Y.-T.; Hsiao, Y.-Y.; Doudeva, L.G.; Yuan, H.S.
Deposited on	:	2009-05-25
Resolution	:	1.98 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 (i) symbol.

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

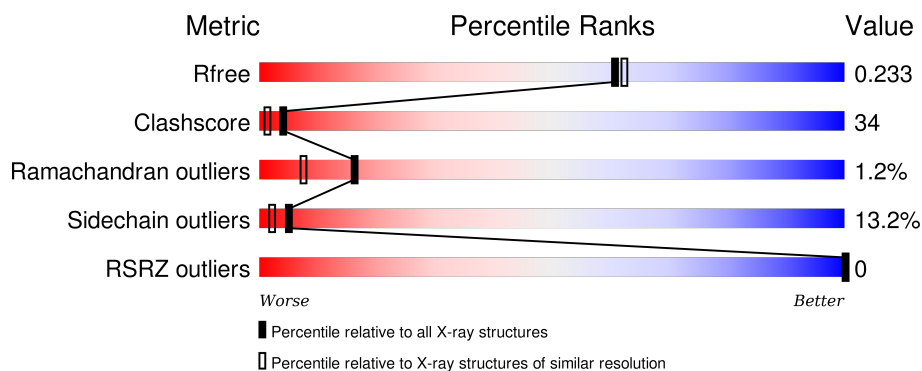|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.98 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		34
Ramachandran outliers		1.2%
Sidechain outliers		13.2%
RSRZ outliers		0

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 <=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	246	44% 35% 5% 16%
1	B	246	44% 35% 7% 13%
1	C	246	41% 30% 8% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5102 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 Os03g0854200 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1575	986	280	298	11			
1	B	213	Total	C	N	O	S	0	0	0
			1625	1015	294	305	11			
1	C	195	Total	C	N	O	S	0	0	0
			1486	935	267	273	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	LEU	-	EXPRESSION TAG	UNP Q84T68
A	240	GLU	-	EXPRESSION TAG	UNP Q84T68
A	241	HIS	-	EXPRESSION TAG	UNP Q84T68
A	242	HIS	-	EXPRESSION TAG	UNP Q84T68
A	243	HIS	-	EXPRESSION TAG	UNP Q84T68
A	244	HIS	-	EXPRESSION TAG	UNP Q84T68
A	245	HIS	-	EXPRESSION TAG	UNP Q84T68
A	246	HIS	-	EXPRESSION TAG	UNP Q84T68
B	239	LEU	-	EXPRESSION TAG	UNP Q84T68
B	240	GLU	-	EXPRESSION TAG	UNP Q84T68
B	241	HIS	-	EXPRESSION TAG	UNP Q84T68
B	242	HIS	-	EXPRESSION TAG	UNP Q84T68
B	243	HIS	-	EXPRESSION TAG	UNP Q84T68
B	244	HIS	-	EXPRESSION TAG	UNP Q84T68
B	245	HIS	-	EXPRESSION TAG	UNP Q84T68
B	246	HIS	-	EXPRESSION TAG	UNP Q84T68
C	239	LEU	-	EXPRESSION TAG	UNP Q84T68
C	240	GLU	-	EXPRESSION TAG	UNP Q84T68
C	241	HIS	-	EXPRESSION TAG	UNP Q84T68
C	242	HIS	-	EXPRESSION TAG	UNP Q84T68
C	243	HIS	-	EXPRESSION TAG	UNP Q84T68
C	244	HIS	-	EXPRESSION TAG	UNP Q84T68
C	245	HIS	-	EXPRESSION TAG	UNP Q84T68

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Chain	Residue	Modelled	Actual	Comment	Reference
C	246	HIS	-	EXPRESSION TAG	UNP Q84T68

- Molecule 2 is water.

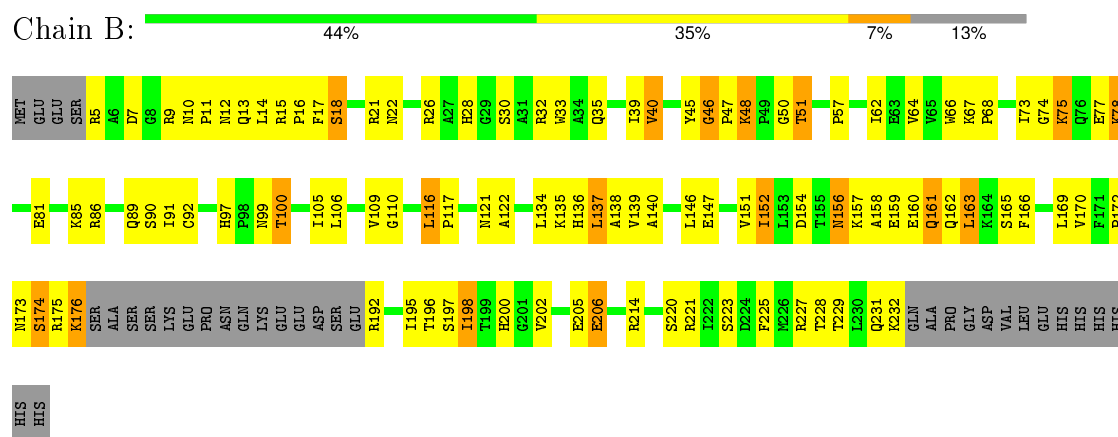| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	152	Total 152	O 152	0	0
2	B	163	Total 163	O 163	0	0
2	C	101	Total 101	O 101	0	0

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.
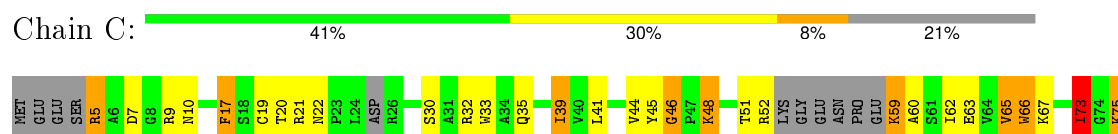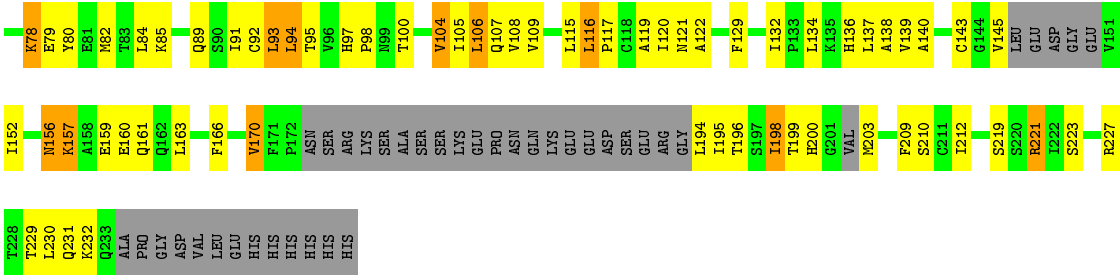
- Molecule 1: Os03g0854200 protein

- Molecule 1: Os03g0854200 protein

- Molecule 1: Os03g0854200 protein

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	111.61Å 111.61Å 57.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.81 – 1.98 26.81 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (26.81-1.98) 98.5 (26.81-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.169 , 0.235 0.169 , 0.233	Depositor DCC
R_{free} test set	2779 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.2	EDS
Estimated twinning fraction	0.501 for h,-h-k,-l 0.069 for -h,-k,l 0.477 for h,-h-k,-l 0.067 for -k,-h,-l	Xtriage
Reported twinning fraction	0.501 for h,-h-k,-l	Depositor
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.24$	Xtriage
Outliers	0 of 55488 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5102	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.33	0/1602	0.56	0/2171
1	B	0.34	0/1652	0.55	0/2234
1	C	0.32	0/1508	0.57	0/2036
All	All	0.33	0/4762	0.56	0/6441

There are no bond length outliers.

There are no bond angle outliers.

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	1575	0	1588	111	0
1	B	1625	0	1648	118	0
1	C	1486	0	1515	95	0
2	A	152	0	0	8	1
2	B	163	0	0	13	0
2	C	101	0	0	3	0
All	All	5102	0	4751	321	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 34.

All (321) 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:121:ASN:HD21	1:A:140:ALA:H	1.12	0.96
1:A:22:ASN:HB3	1:A:129:PHE:CE2	2.02	0.95
1:C:121:ASN:HD21	1:C:140:ALA:H	1.12	0.94
1:B:198:ILE:HD11	1:B:200:HIS:CE1	2.01	0.93
1:C:97:HIS:CD2	1:C:100:THR:HB	2.04	0.93
1:A:15:ARG:HD2	1:A:154:ASP:OD2	1.68	0.93
1:B:62:ILE:HD12	1:B:89:GLN:HA	1.51	0.91
1:A:33:TRP:HE1	1:A:35:GLN:HE21	1.17	0.91
1:C:170:VAL:HG13	1:C:196:THR:HB	1.52	0.91
1:A:94:LEU:HD13	1:A:94:LEU:H	1.37	0.88
1:B:175:ARG:HB2	1:B:176:LYS:HD2	1.54	0.88
1:C:75:LYS:H	1:C:75:LYS:HD3	1.38	0.87
1:A:11:PRO:HB2	1:A:214:ARG:HH22	1.40	0.87
1:C:221:ARG:HG2	1:C:221:ARG:HH11	1.39	0.85
1:B:33:TRP:HE1	1:B:35:GLN:HE21	1.22	0.83
1:C:159:GLU:O	1:C:163:LEU:HD13	1.80	0.81
1:A:145:VAL:HB	1:A:165:SER:HB2	1.63	0.81
1:B:121:ASN:HD21	1:B:140:ALA:H	1.29	0.80
1:B:15:ARG:HD3	1:B:154:ASP:OD2	1.83	0.79
1:B:97:HIS:O	1:B:100:THR:HB	1.83	0.79
1:C:97:HIS:HD2	1:C:100:THR:HB	1.45	0.78
1:C:231:GLN:O	1:C:231:GLN:HG3	1.83	0.78
1:C:20:THR:HG22	1:C:32:ARG:HB3	1.65	0.78
1:B:5:ARG:HD2	1:B:159:GLU:OE2	1.83	0.77
1:B:196:THR:HG22	1:B:197:SER:H	1.48	0.77
1:B:32:ARG:HG2	1:B:39:ILE:HD11	1.67	0.75
1:C:65:VAL:HG13	1:C:105:ILE:HG12	1.68	0.75
1:A:12:ASN:HB3	1:A:214:ARG:HH21	1.52	0.74
1:A:76:GLN:O	1:A:79:GLU:HG2	1.87	0.74
1:A:29:GLY:HA2	1:A:129:PHE:HD2	1.52	0.74
1:B:9:ARG:HA	1:B:13:GLN:HE21	1.51	0.73
1:C:59:LYS:HD3	1:C:59:LYS:N	2.03	0.73
1:B:206:GLU:HB2	2:B:340:HOH:O	1.88	0.73
1:C:33:TRP:HB3	1:C:122:ALA:HB2	1.70	0.73
1:B:136:HIS:CB	1:B:174:SER:HA	2.19	0.72
1:C:21:ARG:HH12	1:C:232:LYS:HB3	1.54	0.72
1:C:39:ILE:HG12	1:C:109:VAL:HB	1.72	0.72
1:C:170:VAL:HG22	1:C:195:ILE:HB	1.72	0.71
1:B:165:SER:HB3	1:B:202:VAL:O	1.90	0.71
1:C:116:LEU:HB3	1:C:117:PRO:HD3	1.72	0.71
1:C:93:LEU:HD12	1:C:95:THR:HG22	1.72	0.70
1:A:45:TYR:O	1:A:46:GLY:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:HB3	1:A:214:ARG:NH2	2.07	0.70
1:A:143:CYS:O	1:A:166:PHE:HB2	1.90	0.70
1:A:22:ASN:CB	1:A:129:PHE:CE2	2.75	0.69
1:A:29:GLY:HA2	1:A:129:PHE:CD2	2.27	0.69
1:B:75:LYS:HE3	1:B:75:LYS:O	1.91	0.69
1:B:176:LYS:H	1:B:176:LYS:CE	2.06	0.69
1:B:170:VAL:HG13	1:B:195:ILE:HB	1.75	0.69
1:B:136:HIS:HB3	1:B:174:SER:HA	1.75	0.69
1:C:67:LYS:HB3	1:C:67:LYS:HZ3	1.57	0.69
1:A:170:VAL:HG22	1:A:195:ILE:HB	1.74	0.68
1:C:156:ASN:HD21	1:C:159:GLU:HG3	1.58	0.68
1:B:161:GLN:HA	1:B:161:GLN:HE21	1.57	0.68
1:C:209:PHE:O	1:C:212:ILE:HG12	1.93	0.68
1:C:19:CYS:HB3	1:C:230:LEU:HD11	1.76	0.68
1:C:97:HIS:HD2	1:C:100:THR:CB	2.07	0.67
1:C:84:LEU:HD21	1:C:106:LEU:HD11	1.75	0.67
1:A:121:ASN:ND2	1:A:140:ALA:H	1.88	0.67
1:A:146:LEU:HB2	1:A:150:GLU:HB2	1.76	0.67
1:A:22:ASN:HB2	2:A:252:HOH:O	1.96	0.67
1:C:78:LYS:HG2	1:C:79:GLU:N	2.09	0.66
1:C:170:VAL:CG1	1:C:196:THR:HB	2.25	0.66
1:B:90:SER:O	1:B:135:LYS:HD2	1.96	0.66
1:A:21:ARG:HE	1:A:21:ARG:HA	1.60	0.66
1:B:116:LEU:HB3	1:B:117:PRO:HD3	1.78	0.66
1:A:15:ARG:CD	1:A:154:ASP:OD2	2.43	0.66
1:A:161:GLN:HG3	1:A:161:GLN:O	1.95	0.66
1:C:221:ARG:CG	1:C:221:ARG:HH11	2.07	0.65
1:B:10:ASN:H	1:B:13:GLN:NE2	1.94	0.65
1:A:66:TRP:CH2	1:A:108:VAL:HG21	2.30	0.65
1:B:147:GLU:CD	1:B:147:GLU:H	2.00	0.65
1:C:157:LYS:O	1:C:161:GLN:HG2	1.97	0.65
1:A:12:ASN:HB3	1:A:214:ARG:HE	1.61	0.65
1:B:32:ARG:CG	1:B:39:ILE:HD11	2.28	0.64
1:B:75:LYS:HE2	2:B:357:HOH:O	1.98	0.63
1:C:33:TRP:HE1	1:C:35:GLN:HE21	1.44	0.62
1:C:106:LEU:CD2	1:C:119:ALA:HB1	2.29	0.62
1:B:198:ILE:HD11	1:B:200:HIS:NE2	2.14	0.62
1:B:17:PHE:HE2	1:B:225:PHE:CD2	2.16	0.62
1:B:198:ILE:HG13	1:B:198:ILE:O	1.98	0.62
1:C:75:LYS:N	1:C:75:LYS:HD3	2.11	0.62
1:A:121:ASN:HD21	1:A:140:ALA:N	1.93	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:THR:HG22	1:B:197:SER:N	2.14	0.62
1:A:15:ARG:HG3	1:A:36:GLY:N	2.15	0.62
1:C:59:LYS:HG2	1:C:98:PRO:HB3	1.82	0.62
1:A:39:ILE:HG12	1:A:109:VAL:HB	1.81	0.61
1:B:62:ILE:HD11	1:B:92:CYS:HB2	1.82	0.61
1:C:22:ASN:HD21	1:C:129:PHE:HB3	1.65	0.61
1:B:91:ILE:HG21	1:B:138:ALA:HB2	1.82	0.61
1:A:55:GLU:O	1:A:57:PRO:HD2	2.01	0.61
1:A:40:VAL:HG11	1:A:106:LEU:HD21	1.82	0.61
1:B:172:PRO:HB2	1:B:174:SER:OG	2.00	0.61
1:C:84:LEU:HD21	1:C:106:LEU:HD21	1.82	0.61
1:A:94:LEU:HD12	2:A:250:HOH:O	2.00	0.61
1:A:12:ASN:HB3	1:A:214:ARG:NE	2.15	0.61
1:B:51:THR:HG22	1:B:99:ASN:ND2	2.16	0.60
1:A:94:LEU:CD1	1:A:94:LEU:H	2.13	0.60
1:B:21:ARG:NE	2:B:372:HOH:O	2.32	0.60
1:C:121:ASN:ND2	1:C:140:ALA:H	1.91	0.60
1:A:56:ASN:O	1:A:56:ASN:OD1	2.19	0.60
1:A:21:ARG:HD3	1:A:129:PHE:CD1	2.36	0.59
1:A:56:ASN:O	1:A:58:GLU:N	2.34	0.59
1:C:62:ILE:HD12	1:C:89:GLN:HA	1.82	0.59
1:B:35:GLN:HG2	2:B:256:HOH:O	2.02	0.59
1:B:160:GLU:HA	1:B:166:PHE:CE1	2.38	0.59
1:A:32:ARG:NH1	2:A:276:HOH:O	2.36	0.58
1:B:48:LYS:HG2	2:B:305:HOH:O	2.04	0.58
1:A:20:THR:HG23	1:A:32:ARG:HB3	1.85	0.58
1:A:40:VAL:CG1	1:A:106:LEU:HD21	2.34	0.58
1:C:160:GLU:HA	1:C:163:LEU:HD22	1.86	0.58
1:B:39:ILE:HG13	1:B:109:VAL:HB	1.86	0.58
1:B:64:VAL:HB	1:B:85:LYS:HG2	1.86	0.58
1:A:51:THR:HG22	1:A:55:GLU:HB2	1.86	0.58
1:C:52:ARG:HA	1:C:52:ARG:CZ	2.33	0.58
1:C:22:ASN:HD22	1:C:30:SER:H	1.52	0.58
1:A:86:ARG:HH11	1:A:86:ARG:HB2	1.69	0.58
1:B:176:LYS:H	1:B:176:LYS:CD	2.17	0.57
1:C:106:LEU:HD12	1:C:106:LEU:N	2.18	0.57
1:C:48:LYS:NZ	1:C:48:LYS:HA	2.18	0.57
1:C:156:ASN:ND2	1:C:159:GLU:H	2.02	0.57
1:B:22:ASN:HD22	1:B:30:SER:H	1.52	0.57
1:C:21:ARG:HG3	2:C:327:HOH:O	2.04	0.57
1:A:51:THR:HB	1:A:57:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:THR:HG23	2:C:283:HOH:O	2.03	0.57
1:A:66:TRP:HB2	1:A:81:GLU:HB2	1.87	0.57
1:B:16:PRO:HD3	2:B:268:HOH:O	2.04	0.57
1:C:20:THR:CG2	1:C:32:ARG:HB3	2.34	0.57
1:C:66:TRP:HE1	1:C:84:LEU:HD22	1.69	0.57
1:A:66:TRP:CZ3	1:A:77:GLU:HB3	2.39	0.57
1:B:48:LYS:HD3	2:B:353:HOH:O	2.05	0.56
1:B:169:LEU:HD23	1:B:197:SER:HB2	1.85	0.56
1:C:62:ILE:HD11	1:C:94:LEU:HD11	1.87	0.56
1:C:198:ILE:HG12	1:C:198:ILE:O	2.05	0.56
1:B:17:PHE:HE2	1:B:225:PHE:CG	2.23	0.56
1:C:48:LYS:HZ3	1:C:48:LYS:HA	1.69	0.56
1:C:67:LYS:HZ2	1:C:107:GLN:HE22	1.53	0.56
1:B:18:SER:HB2	2:B:250:HOH:O	2.05	0.56
1:C:166:PHE:CE1	1:C:200:HIS:HB2	2.41	0.56
1:C:67:LYS:HB3	1:C:67:LYS:NZ	2.21	0.55
1:A:116:LEU:O	1:A:120:ILE:HG13	2.06	0.55
1:B:33:TRP:HB3	1:B:122:ALA:HB2	1.88	0.55
1:C:67:LYS:HB2	1:C:107:GLN:HA	1.88	0.55
1:C:84:LEU:CD2	1:C:106:LEU:HD11	2.37	0.55
1:B:161:GLN:HA	1:B:161:GLN:NE2	2.22	0.55
1:A:21:ARG:NE	1:A:21:ARG:HA	2.22	0.55
1:B:173:ASN:HD21	1:B:227:ARG:CZ	2.20	0.55
1:B:74:GLY:O	1:B:78:LYS:HB2	2.07	0.55
1:C:73:ILE:H	1:C:73:ILE:HD12	1.71	0.54
1:C:75:LYS:HA	1:C:78:LYS:HD3	1.89	0.54
1:A:66:TRP:CE3	1:A:77:GLU:HB3	2.42	0.54
1:C:67:LYS:O	1:C:108:VAL:HG23	2.07	0.54
1:B:176:LYS:H	1:B:176:LYS:HE2	1.71	0.54
1:A:12:ASN:HB3	1:A:214:ARG:CZ	2.38	0.54
1:B:40:VAL:CG2	1:B:106:LEU:HD11	2.38	0.54
1:A:91:ILE:HG21	1:A:138:ALA:HB2	1.89	0.54
1:B:51:THR:HG21	1:B:57:PRO:HG3	1.90	0.54
1:C:65:VAL:CG1	1:C:105:ILE:HG12	2.38	0.53
1:B:28:HIS:ND1	1:B:46:GLY:N	2.54	0.53
1:C:41:LEU:HB3	1:C:107:GLN:HB3	1.89	0.53
1:B:160:GLU:HA	1:B:166:PHE:CZ	2.44	0.53
1:C:91:ILE:HG21	1:C:138:ALA:HB2	1.89	0.53
1:A:73:ILE:HG13	1:A:77:GLU:HB2	1.90	0.53
1:B:139:VAL:HG21	1:B:223:SER:OG	2.09	0.53
1:C:84:LEU:CD2	1:C:106:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:HG23	1:A:86:ARG:NH1	2.24	0.53
1:C:21:ARG:NH1	1:C:232:LYS:HB3	2.24	0.52
1:B:22:ASN:ND2	1:B:30:SER:H	2.06	0.52
1:C:5:ARG:O	1:C:5:ARG:HG2	2.08	0.52
1:C:33:TRP:CB	1:C:122:ALA:HB2	2.40	0.52
1:C:45:TYR:O	1:C:46:GLY:O	2.28	0.52
1:A:28:HIS:HB2	1:A:46:GLY:H	1.75	0.52
1:A:33:TRP:HE1	1:A:35:GLN:NE2	1.98	0.51
1:A:159:GLU:O	1:A:163:LEU:HD13	2.10	0.51
1:A:173:ASN:ND2	1:A:227:ARG:HH12	2.09	0.51
1:A:227:ARG:HG3	1:A:227:ARG:HH11	1.76	0.51
1:B:86:ARG:HD3	2:B:255:HOH:O	2.09	0.51
1:B:39:ILE:HG23	1:B:110:GLY:N	2.26	0.51
1:C:75:LYS:O	1:C:79:GLU:HG2	2.10	0.51
1:B:9:ARG:HA	1:B:13:GLN:NE2	2.23	0.51
1:B:136:HIS:HB2	1:B:174:SER:HA	1.93	0.50
1:B:170:VAL:HG22	1:B:195:ILE:HD12	1.92	0.50
1:A:82:MET:SD	1:A:86:ARG:HD3	2.50	0.50
1:C:17:PHE:CD1	1:C:17:PHE:N	2.79	0.50
1:A:66:TRP:HH2	1:A:115:LEU:HD21	1.75	0.50
1:A:83:THR:HG23	1:A:86:ARG:HH12	1.76	0.50
1:C:156:ASN:ND2	1:C:159:GLU:HG3	2.26	0.50
1:B:192:ARG:NH2	1:B:195:ILE:HA	2.27	0.50
1:B:146:LEU:HD23	1:B:163:LEU:HD11	1.94	0.50
1:B:231:GLN:O	1:B:232:LYS:CB	2.60	0.49
1:B:156:ASN:ND2	1:B:159:GLU:H	2.10	0.49
1:B:231:GLN:O	1:B:232:LYS:HB3	2.13	0.49
1:A:153:LEU:HD11	1:A:214:ARG:HG3	1.94	0.49
1:B:86:ARG:HB3	1:B:86:ARG:CZ	2.41	0.49
1:A:9:ARG:NH1	1:A:15:ARG:HB3	2.27	0.49
1:B:176:LYS:N	1:B:176:LYS:CD	2.76	0.49
1:A:73:ILE:HD11	1:A:77:GLU:O	2.13	0.49
1:B:86:ARG:CZ	1:B:86:ARG:CB	2.91	0.49
1:C:223:SER:O	1:C:227:ARG:HG3	2.13	0.49
1:C:66:TRP:HH2	1:C:115:LEU:HG	1.77	0.49
1:A:17:PHE:HA	1:A:34:ALA:O	2.13	0.48
1:B:17:PHE:CE2	1:B:225:PHE:CD2	3.00	0.48
1:A:11:PRO:HB2	1:A:214:ARG:NH2	2.20	0.48
1:B:39:ILE:HD12	1:B:40:VAL:H	1.77	0.48
1:C:91:ILE:CG2	1:C:195:ILE:HD13	2.43	0.48
1:C:203:MET:N	2:C:265:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ALA:HB3	2:A:389:HOH:O	2.14	0.48
1:B:176:LYS:N	1:B:176:LYS:HD2	2.29	0.47
1:A:221:ARG:HD3	2:A:329:HOH:O	2.14	0.47
1:A:29:GLY:CA	1:A:129:PHE:HD2	2.25	0.47
1:C:221:ARG:CG	1:C:221:ARG:NH1	2.71	0.47
1:A:169:LEU:HD23	1:A:197:SER:HB2	1.96	0.47
1:B:137:LEU:HB2	1:B:173:ASN:HB3	1.95	0.47
1:B:156:ASN:HD21	1:B:158:ALA:HB3	1.79	0.47
1:B:192:ARG:HH21	1:B:195:ILE:HG12	1.80	0.47
1:B:68:PRO:HB3	1:B:77:GLU:OE2	2.14	0.47
1:B:62:ILE:CD1	1:B:89:GLN:HA	2.35	0.47
1:A:56:ASN:C	1:A:58:GLU:H	2.17	0.47
1:B:228:THR:HG22	1:B:229:THR:N	2.30	0.47
1:A:12:ASN:CB	1:A:214:ARG:HH21	2.26	0.47
1:B:156:ASN:HD22	1:B:156:ASN:C	2.19	0.47
1:B:172:PRO:HG2	1:B:192:ARG:HB3	1.97	0.47
1:A:20:THR:CG2	1:A:32:ARG:HB3	2.45	0.47
1:C:73:ILE:CD1	1:C:73:ILE:H	2.28	0.47
1:B:17:PHE:CE2	1:B:225:PHE:CG	3.02	0.46
1:B:221:ARG:NH1	2:B:321:HOH:O	2.49	0.46
1:C:121:ASN:HD21	1:C:140:ALA:N	1.95	0.46
1:B:66:TRP:HB2	1:B:81:GLU:HG3	1.97	0.46
1:B:157:LYS:HG3	2:B:307:HOH:O	2.15	0.46
1:B:10:ASN:HB3	1:B:11:PRO:HD2	1.98	0.46
1:A:88:LEU:HD22	1:A:127:LEU:HD11	1.98	0.46
1:B:175:ARG:HE	1:B:227:ARG:HH22	1.64	0.46
1:A:195:ILE:HG22	1:A:196:THR:HG23	1.98	0.46
1:A:7:ASP:OD2	1:A:9:ARG:HG3	2.16	0.46
1:A:91:ILE:HG22	1:A:195:ILE:HD13	1.97	0.46
1:A:116:LEU:HB3	1:A:117:PRO:HD3	1.97	0.46
1:C:156:ASN:C	1:C:156:ASN:HD22	2.19	0.45
1:A:82:MET:SD	1:A:86:ARG:CD	3.04	0.45
1:A:198:ILE:HD11	1:B:202:VAL:CG2	2.46	0.45
1:A:83:THR:HA	1:A:86:ARG:HH11	1.82	0.45
1:C:139:VAL:HG11	1:C:219:SER:HB2	1.99	0.45
1:A:22:ASN:HB3	1:A:129:PHE:CD2	2.49	0.45
1:B:169:LEU:HD23	1:B:197:SER:CB	2.46	0.45
1:C:22:ASN:ND2	1:C:30:SER:H	2.15	0.45
1:C:97:HIS:CD2	1:C:100:THR:CB	2.85	0.45
1:A:30:SER:HA	1:A:42:ALA:O	2.17	0.45
1:B:192:ARG:NH2	1:B:195:ILE:HG12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:CYS:O	1:C:166:PHE:HB2	2.16	0.45
1:B:9:ARG:CA	1:B:13:GLN:HE21	2.24	0.45
1:A:66:TRP:CH2	1:A:108:VAL:CG2	2.97	0.45
1:A:209:PHE:O	1:A:212:ILE:HG12	2.17	0.45
1:C:157:LYS:HB2	1:C:157:LYS:HE3	1.62	0.44
1:C:116:LEU:O	1:C:120:ILE:HG13	2.18	0.44
1:C:67:LYS:HD2	1:C:67:LYS:HA	1.84	0.44
1:B:175:ARG:HH21	1:B:227:ARG:HH22	1.65	0.44
1:A:145:VAL:N	1:A:163:LEU:HD23	2.32	0.44
1:B:192:ARG:NH2	2:B:285:HOH:O	2.49	0.44
1:A:96:VAL:C	1:A:98:PRO:HD3	2.37	0.44
1:C:80:TYR:CD1	1:C:116:LEU:HG	2.52	0.44
1:A:33:TRP:HB3	1:A:122:ALA:HB2	1.99	0.44
1:C:75:LYS:H	1:C:75:LYS:CD	2.10	0.44
1:C:7:ASP:OD1	1:C:9:ARG:HD3	2.18	0.44
1:A:22:ASN:CG	1:A:129:PHE:CZ	2.91	0.44
1:B:66:TRP:O	1:B:73:ILE:HD12	2.17	0.44
1:A:165:SER:O	1:A:166:PHE:HB3	2.17	0.44
1:C:85:LYS:NZ	1:C:89:GLN:HE21	2.16	0.44
1:A:56:ASN:O	1:A:56:ASN:CG	2.56	0.44
1:B:68:PRO:HG3	1:B:73:ILE:HA	1.99	0.44
1:B:15:ARG:NH1	1:B:154:ASP:OD1	2.51	0.43
1:B:163:LEU:HB3	1:B:166:PHE:CZ	2.53	0.43
1:B:151:VAL:O	1:B:214:ARG:NH1	2.51	0.43
1:A:10:ASN:HB2	1:A:11:PRO:HD2	2.00	0.43
1:B:195:ILE:O	1:B:196:THR:OG1	2.30	0.43
1:B:169:LEU:CD2	1:B:197:SER:HB2	2.48	0.43
1:A:75:LYS:HB2	1:A:75:LYS:HE2	1.91	0.43
1:A:40:VAL:HG13	1:A:106:LEU:CD2	2.49	0.43
1:B:62:ILE:HD11	1:B:92:CYS:CB	2.49	0.43
1:A:143:CYS:O	1:A:166:PHE:CB	2.65	0.42
1:B:5:ARG:HA	2:B:407:HOH:O	2.19	0.42
1:C:60:ALA:O	1:C:94:LEU:HG	2.19	0.42
1:A:194:LEU:HD11	1:B:205:GLU:OE1	2.20	0.42
1:C:67:LYS:NZ	1:C:107:GLN:HE22	2.16	0.42
1:C:44:VAL:HG22	1:C:104:VAL:HB	2.01	0.42
1:B:156:ASN:HD22	1:B:158:ALA:N	2.18	0.42
1:A:194:LEU:C	1:A:194:LEU:HD12	2.39	0.42
1:A:67:LYS:HA	1:A:68:PRO:HD3	1.84	0.42
1:A:168:HIS:HB2	1:A:198:ILE:HG23	2.02	0.42
1:A:144:GLY:HA2	1:A:166:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:ND2	2:A:298:HOH:O	2.52	0.41
1:C:92:CYS:HB3	1:C:94:LEU:HD13	2.01	0.41
1:B:152:ILE:HG22	1:B:152:ILE:O	2.20	0.41
1:A:161:GLN:NE2	1:C:166:PHE:CD1	2.88	0.41
1:B:50:GLY:HA2	1:B:99:ASN:HD21	1.85	0.41
1:A:154:ASP:HB3	2:A:280:HOH:O	2.20	0.41
1:B:47:PRO:HB3	1:B:100:THR:HG21	2.02	0.41
1:A:22:ASN:ND2	1:A:129:PHE:CZ	2.88	0.41
1:B:176:LYS:H	1:B:176:LYS:HD2	1.84	0.41
1:A:166:PHE:CE2	1:A:200:HIS:HB2	2.56	0.41
1:A:51:THR:HG21	1:A:57:PRO:HD3	2.03	0.41
1:A:87:THR:O	1:A:90:SER:HB3	2.20	0.41
1:B:196:THR:CG2	1:B:197:SER:H	2.24	0.41
1:C:52:ARG:NH1	1:C:63:GLU:OE2	2.54	0.41
1:A:21:ARG:CZ	1:A:129:PHE:HB2	2.50	0.41
1:B:40:VAL:HG21	1:B:106:LEU:HD11	2.03	0.41
1:B:50:GLY:HA2	1:B:99:ASN:ND2	2.36	0.41
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.87	0.41
1:C:139:VAL:HG21	1:C:223:SER:HB3	2.03	0.41
1:B:67:LYS:HA	1:B:68:PRO:HD2	1.91	0.41
1:B:45:TYR:CE2	1:B:105:ILE:HD12	2.56	0.41
1:C:82:MET:HA	1:C:82:MET:HE2	2.03	0.41
1:B:223:SER:HB3	1:B:227:ARG:HH11	1.86	0.41
1:B:45:TYR:HE2	1:B:105:ILE:HD12	1.84	0.41
1:C:132:ILE:O	1:C:134:LEU:HD13	2.21	0.41
1:A:56:ASN:O	1:A:58:GLU:HG2	2.20	0.40
1:A:23:PRO:HD2	1:A:30:SER:OG	2.21	0.40
1:B:78:LYS:HD2	1:B:78:LYS:O	2.21	0.40
1:A:53:LYS:N	2:A:302:HOH:O	2.46	0.40
1:A:39:ILE:HG13	1:A:40:VAL:N	2.36	0.40
1:A:59:LYS:HG2	1:A:94:LEU:HD23	2.03	0.40
1:A:94:LEU:HD22	1:A:95:THR:N	2.37	0.40
1:B:7:ASP:CG	1:B:9:ARG:HD3	2.41	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)
2:A:362:HOH:O	2:A:366:HOH:O[3_554]	2.05	0.15

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	203/246 (82%)	190 (94%)	9 (4%)	4 (2%)	9	3
1	B	209/246 (85%)	200 (96%)	8 (4%)	1 (0%)	34	25
1	C	183/246 (74%)	172 (94%)	9 (5%)	2 (1%)	17	8
All	All	595/738 (81%)	562 (94%)	26 (4%)	7 (1%)	16	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	PRO
1	C	46	GLY
1	A	46	GLY
1	B	46	GLY
1	A	52	ARG
1	C	73	ILE
1	A	56	ASN

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	173/208 (83%)	157 (91%)	16 (9%)	11	5
1	B	178/208 (86%)	155 (87%)	23 (13%)	5	2
1	C	163/208 (78%)	134 (82%)	29 (18%)	2	1
All	All	514/624 (82%)	446 (87%)	68 (13%)	5	2

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	20	THR
1	A	26	ARG
1	A	39	ILE
1	A	40	VAL
1	A	51	THR
1	A	65	VAL
1	A	66	TRP
1	A	78	LYS
1	A	94	LEU
1	A	100	THR
1	A	116	LEU
1	A	148	ASP
1	A	152	ILE
1	A	170	VAL
1	A	197	SER
1	B	12	ASN
1	B	14	LEU
1	B	18	SER
1	B	26	ARG
1	B	40	VAL
1	B	48	LYS
1	B	51	THR
1	B	75	LYS
1	B	78	LYS
1	B	100	THR
1	B	116	LEU
1	B	134	LEU
1	B	137	LEU
1	B	152	ILE
1	B	156	ASN
1	B	161	GLN
1	B	162	GLN
1	B	163	LEU
1	B	174	SER
1	B	176	LYS
1	B	198	ILE
1	B	206	GLU
1	B	220	SER
1	C	5	ARG
1	C	10	ASN
1	C	17	PHE

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Mol	Chain	Res	Type
1	C	39	ILE
1	C	48	LYS
1	C	51	THR
1	C	59	LYS
1	C	65	VAL
1	C	66	TRP
1	C	73	ILE
1	C	75	LYS
1	C	78	LYS
1	C	93	LEU
1	C	94	LEU
1	C	104	VAL
1	C	106	LEU
1	C	116	LEU
1	C	136	HIS
1	C	137	LEU
1	C	145	VAL
1	C	152	ILE
1	C	156	ASN
1	C	157	LYS
1	C	170	VAL
1	C	194	LEU
1	C	198	ILE
1	C	210	SER
1	C	221	ARG
1	C	229	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	56	ASN
1	A	99	ASN
1	A	107	GLN
1	A	121	ASN
1	A	161	GLN
1	A	173	ASN
1	B	10	ASN
1	B	12	ASN
1	B	13	GLN
1	B	22	ASN
1	B	35	GLN

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Mol	Chain	Res	Type
1	B	56	ASN
1	B	99	ASN
1	B	107	GLN
1	B	121	ASN
1	B	156	ASN
1	B	161	GLN
1	B	162	GLN
1	B	168	HIS
1	B	173	ASN
1	C	12	ASN
1	C	22	ASN
1	C	35	GLN
1	C	89	GLN
1	C	97	HIS
1	C	107	GLN
1	C	121	ASN
1	C	136	HIS
1	C	156	ASN
1	C	233	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	207/246 (84%)	-0.38	0	100	100	16, 24, 32, 38	0
1	B	213/246 (86%)	-0.40	0	100	100	17, 24, 33, 36	0
1	C	195/246 (79%)	-0.31	0	100	100	22, 28, 34, 41	0
All	All	615/738 (83%)	-0.36	0	100	100	16, 25, 34, 41	0

There are no RSRZ outliers to report.

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.