Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 02:00 AM EDT

PDB ID	:	4I43
Title	:	Crystal structure of Prp8:Aar2 complex
Authors	:	Galej, W.P.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on	:	2012-11-27
Resolution	:	2.00 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 (1)) were used in the production of this report:

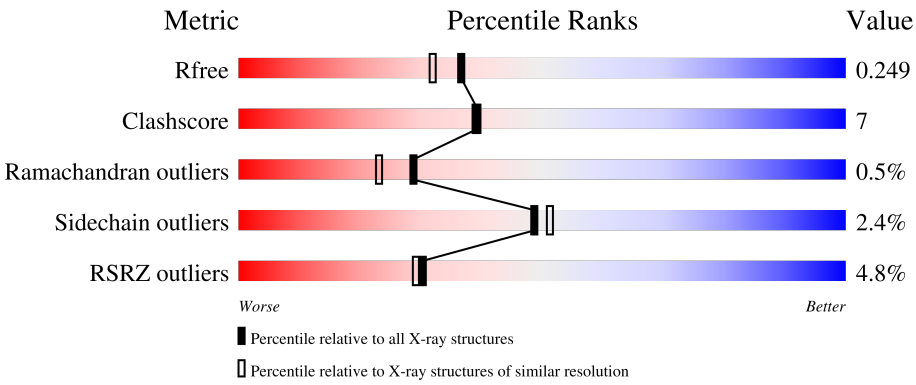
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	384	6% 72% 14% • 13%
2	B	1564	4% 74% 14% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14902 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 A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2751	1754	447	533	17	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ALA	-	expression tag	UNP P32357
A	357	ALA	-	expression tag	UNP P32357
A	358	GLY	-	expression tag	UNP P32357
A	359	LYS	-	expression tag	UNP P32357
A	360	VAL	-	expression tag	UNP P32357
A	361	ALA	-	expression tag	UNP P32357
A	362	ARG	-	expression tag	UNP P32357
A	363	GLY	-	expression tag	UNP P32357
A	364	SER	-	expression tag	UNP P32357
A	365	ARG	-	expression tag	UNP P32357
A	366	SER	-	expression tag	UNP P32357
A	367	GLY	-	expression tag	UNP P32357
A	368	SER	-	expression tag	UNP P32357
A	369	GLU	-	expression tag	UNP P32357
A	370	ASN	-	expression tag	UNP P32357
A	371	LEU	-	expression tag	UNP P32357
A	372	TYR	-	expression tag	UNP P32357
A	373	PHE	-	expression tag	UNP P32357
A	374	GLN	-	expression tag	UNP P32357
A	375	GLY	-	expression tag	UNP P32357
A	376	SER	-	expression tag	UNP P32357
A	377	HIS	-	expression tag	UNP P32357
A	378	HIS	-	expression tag	UNP P32357
A	379	HIS	-	expression tag	UNP P32357
A	380	HIS	-	expression tag	UNP P32357
A	381	HIS	-	expression tag	UNP P32357
A	382	HIS	-	expression tag	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
A	383	HIS	-	expression tag	UNP P32357
A	384	HIS	-	expression tag	UNP P32357

- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1407	11481	7384	1936	2124	37	0	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	850	MET	-	expression tag	UNP P33334
B	851	ALA	-	expression tag	UNP P33334
B	852	ARG	-	expression tag	UNP P33334
B	853	ALA	-	expression tag	UNP P33334
B	854	LYS	-	expression tag	UNP P33334
B	855	ARG	-	expression tag	UNP P33334
B	856	ARG	-	expression tag	UNP P33334
B	857	TRP	-	expression tag	UNP P33334
B	858	LYS	-	expression tag	UNP P33334
B	859	LYS	-	expression tag	UNP P33334
B	860	ASN	-	expression tag	UNP P33334
B	861	PHE	-	expression tag	UNP P33334
B	862	ILE	-	expression tag	UNP P33334
B	863	ALA	-	expression tag	UNP P33334
B	864	VAL	-	expression tag	UNP P33334
B	865	SER	-	expression tag	UNP P33334
B	866	ALA	-	expression tag	UNP P33334
B	867	ALA	-	expression tag	UNP P33334
B	868	ASN	-	expression tag	UNP P33334
B	869	ARG	-	expression tag	UNP P33334
B	870	PHE	-	expression tag	UNP P33334
B	871	LYS	-	expression tag	UNP P33334
B	872	LYS	-	expression tag	UNP P33334
B	873	ILE	-	expression tag	UNP P33334
B	874	SER	-	expression tag	UNP P33334
B	875	SER	-	expression tag	UNP P33334
B	876	SER	-	expression tag	UNP P33334
B	877	GLY	-	expression tag	UNP P33334
B	878	ALA	-	expression tag	UNP P33334
B	879	LEU	-	expression tag	UNP P33334

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Chain	Residue	Modelled	Actual	Comment	Reference
B	880	GLY	-	expression tag	UNP P33334
B	881	SER	-	expression tag	UNP P33334
B	882	GLY	-	expression tag	UNP P33334
B	883	SER	-	expression tag	UNP P33334
B	884	GLY	-	expression tag	UNP P33334

- Molecule 3 is water.

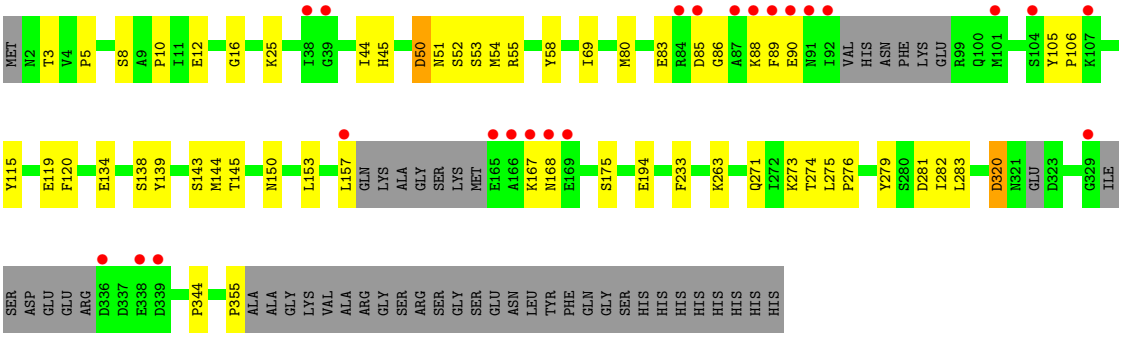
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	156	156	156	0	0
			Total	O		
3	B	514	514	514	0	0

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.

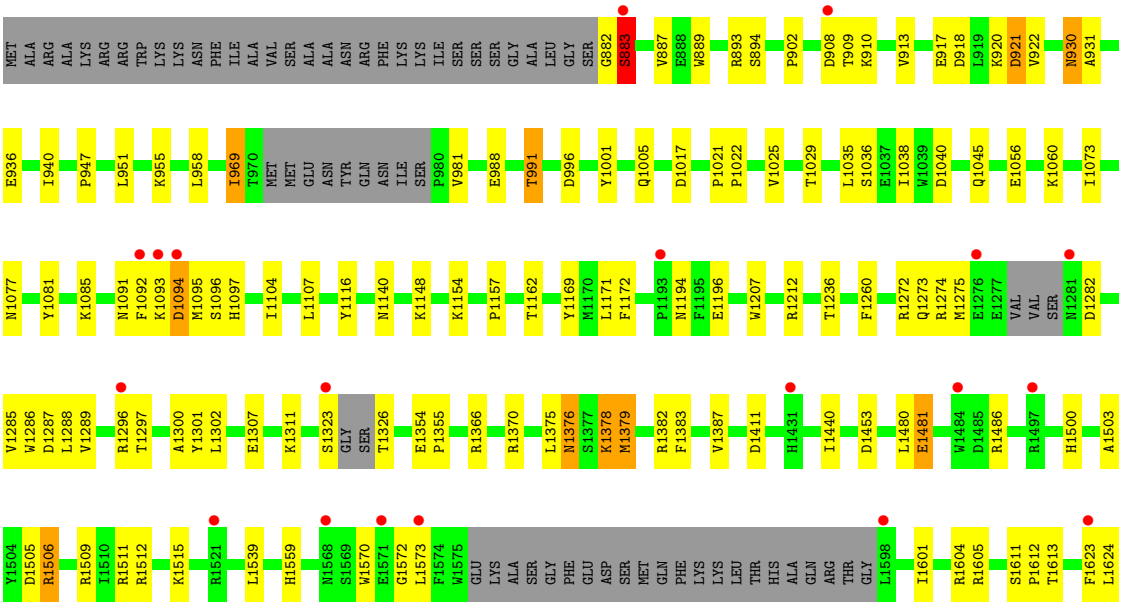
- Molecule 1: A1 cistron-splicing factor AAR2

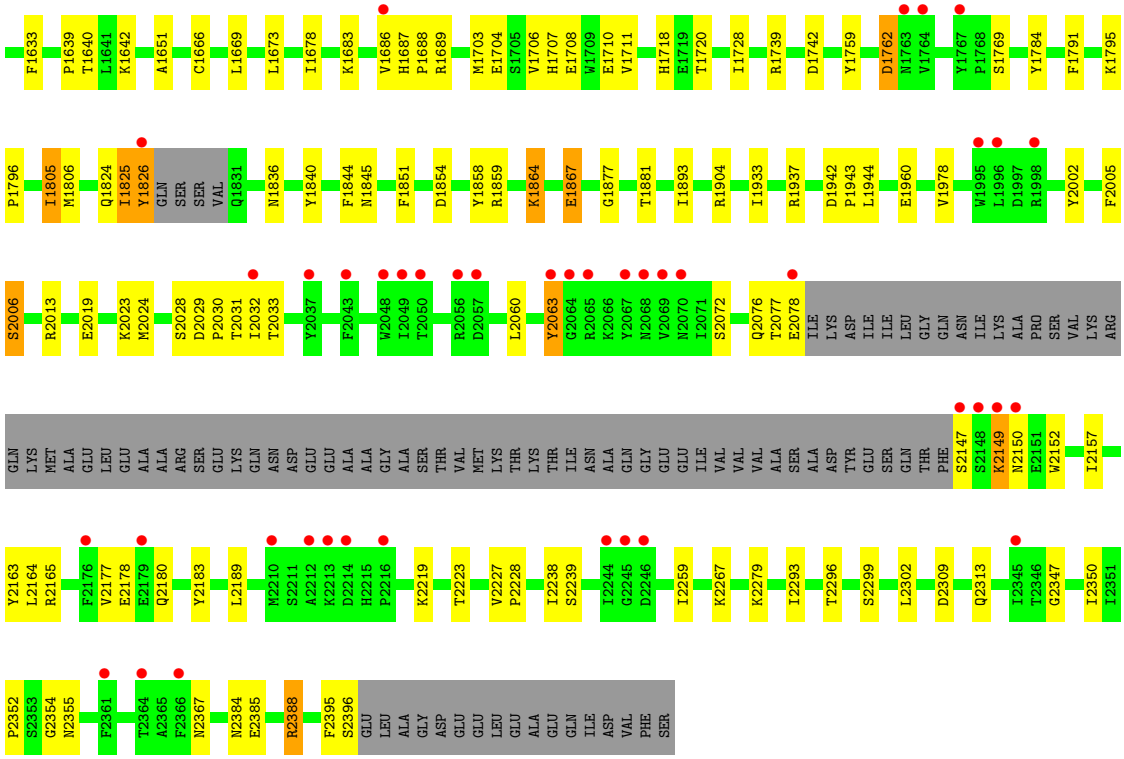
Chain A:



- Molecule 2: Pre-mRNA-splicing factor 8

Chain B:




F1633 P1639 T1640 L1641 K1642 A1651 C1666 L1669 L1673 I1678 K1683 V1686 H1687 P1688 R1689 M1703 E1704 S1705 V1706 H1707 E1708 W1709 E1710 V1711 H1718 E1719 T1720 I1728 R1739 D1742 Y1759 D1762 N1763 V1764 Y1767 P1768 S1769 Y1784 F1791 K1795
P1796 I1805 M1806 Q1824 I1825 Y1826 GLN SER SER VAL Q1831 N1836 Y1840 F1844 N1845 F1851 D1854 Y1858 R1859 K1864 E1867 G1877 T1881 I1893 R1904 I1933 R1937 D1942 P1943 L1944 E1960 V1978 W1995 L1996 D1997 R1998 Y2002 F2005
S2006 R2013 E2019 K2023 M2024 S2028 D2029 P2030 T2031 I2032 T2033 Y2037 F2043 W2048 I2049 T2050 R2056 D2057 L2060 Y2063 G2064 R2065 K2066 Y2067 N2068 V2069 N2070 I2071 S2072 Q2076 T2077 E2078 ILE LYS ASP ILE ILE LEU GLY GLN ASN ILE LYS ALA PRO SER VAL LYS ARG
GLN LYS MET ALA GLU LEU GLU ALA ALA ARG SER GLU LYS GLN ASN ASP GLU GLU ALA ALA GLY ALA SER THR VAL MET LYS THR LYS THR ILE ASN ALA GLN GLY GLU GLU ILE VAL VAL VAL ALA SER ALA ASP TYR GLU SER GLN THR PHE S2147 S2148 K2149 N2150 E2151 W2152 I2157
Y2163 L2164 R2165 F2176 V2177 E2178 E2179 Q2180 Y2183 L2189 W2210 S2211 A2212 K2213 D2214 H2215 P2216 K2219 T2223 V2227 P2228 I2238 S2239 T2244 G2245 D2246 I2259 K2267 K2279 I2293 T2296 S2299 L2302 D2309 Q2313 T2345 T2346 G2347 I2350 I2351
P2352 S2353 G2354 N2355 F2361 T2364 A2365 F2366 N2367 N2384 E2385 R2388 F2395 S2396 GLU LEU ALA GLY ASP GLU GLU LEU GLU ALA GLU GLN ILE ASP VAL PHE SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.86Å 158.59Å 220.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.00 48.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.30-2.00) 100.0 (48.30-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.198 , 0.249 0.202 , 0.249	Depositor DCC
R_{free} test set	7044 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14902	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

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	0.39	0/2818	0.50	0/3806
2	B	0.35	0/11756	0.51	0/15941
All	All	0.36	0/14574	0.51	0/19747

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1825	ILE	Peptide

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	2751	0	2597	41	0
2	B	11481	0	11410	177	0
3	A	156	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	514	0	0	22	1
All	All	14902	0	14007	209	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 7.

All (209) 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)
2:B:1207:TRP:O	2:B:1212:ARG:NH1	2.06	0.89
1:A:282:ILE:HG13	2:B:1604:ARG:HD3	1.56	0.87
2:B:918:ASP:OD1	2:B:1515:LYS:NZ	2.12	0.83
2:B:1091:ASN:OD1	2:B:1096:SER:HB3	1.78	0.82
2:B:1383:PHE:HE2	2:B:1387:VAL:HG21	1.45	0.82
2:B:1017:ASP:HA	2:B:1509:ARG:HG3	1.65	0.79
2:B:1759:TYR:O	2:B:1762:ASP:HB2	1.83	0.78
2:B:1854:ASP:OD1	2:B:1937:ARG:HD3	1.87	0.75
2:B:1383:PHE:CE2	2:B:1387:VAL:HG21	2.21	0.74
2:B:882:GLY:O	2:B:883:SER:HB3	1.86	0.74
1:A:282:ILE:HG13	2:B:1604:ARG:CD	2.17	0.73
2:B:1687:HIS:HD2	2:B:1689:ARG:H	1.39	0.71
2:B:2385:GLU:HG3	2:B:2388:ARG:NH2	2.06	0.70
2:B:2227:VAL:CG1	2:B:2239:SER:OG	2.41	0.69
1:A:145:THR:HG23	2:B:1651:ALA:HB2	1.77	0.66
2:B:1453:ASP:OD2	2:B:1486:ARG:HD2	1.95	0.66
2:B:1718:HIS:CE1	3:B:3002:HOH:O	2.48	0.65
2:B:2149:LYS:HG3	2:B:2150:ASN:N	2.12	0.63
2:B:1025:VAL:O	2:B:1029:THR:HG23	1.99	0.63
2:B:908:ASP:OD1	2:B:951:LEU:HD22	1.99	0.63
2:B:1825:ILE:O	2:B:1826:TYR:CD1	2.52	0.63
2:B:1375:LEU:O	2:B:1376:ASN:HB2	1.98	0.62
2:B:1060:LYS:HG3	3:B:2579:HOH:O	1.99	0.61
3:A:551:HOH:O	2:B:1864:LYS:HE2	2.00	0.61
2:B:1383:PHE:HE2	2:B:1387:VAL:CG2	2.12	0.61
2:B:2077:THR:O	2:B:2078:GLU:CB	2.49	0.60
2:B:913:VAL:O	2:B:917:GLU:HG2	2.02	0.59
2:B:908:ASP:OD2	2:B:951:LEU:HD13	2.03	0.59
2:B:1687:HIS:CD2	2:B:1688:PRO:HD2	2.38	0.58
2:B:889:TRP:O	2:B:893:ARG:HG2	2.03	0.58
2:B:2227:VAL:HG13	2:B:2239:SER:OG	2.03	0.58
1:A:105:TYR:CD1	1:A:106:PRO:HD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:CG2	2:B:1651:ALA:HB2	2.34	0.57
2:B:1669:LEU:HD13	2:B:1703:MET:HE3	1.87	0.57
2:B:2019:GLU:HG2	2:B:2023:LYS:HD2	1.87	0.57
1:A:8:SER:OG	1:A:10:PRO:HD3	2.04	0.57
1:A:139:TYR:CD2	1:A:144:MET:HE1	2.41	0.56
2:B:1505:ASP:OD1	2:B:1511:ARG:NH2	2.38	0.56
1:A:120:PHE:O	3:A:542:HOH:O	2.17	0.56
2:B:883:SER:O	2:B:887:VAL:HG23	2.06	0.56
2:B:1287:ASP:HB3	2:B:1296:ARG:HD2	1.87	0.56
2:B:2077:THR:O	2:B:2078:GLU:HB2	2.05	0.56
2:B:1085:LYS:CE	3:B:2749:HOH:O	2.54	0.56
1:A:115:TYR:O	1:A:119:GLU:N	2.38	0.56
1:A:273:LYS:NZ	3:A:536:HOH:O	2.39	0.55
1:A:355:PRO:HB2	2:B:2267:LYS:HD3	1.89	0.55
1:A:69:ILE:HD13	1:A:80:MET:HA	1.88	0.55
2:B:1370:ARG:NH1	3:B:2966:HOH:O	2.40	0.55
2:B:1559:HIS:HD2	2:B:1613:THR:OG1	1.89	0.55
2:B:1311:LYS:NZ	3:B:2818:HOH:O	2.38	0.54
2:B:2076:GLN:N	2:B:2076:GLN:OE1	2.40	0.54
2:B:1378:LYS:HE2	2:B:1623:PHE:HE2	1.73	0.54
2:B:1687:HIS:CD2	2:B:1689:ARG:H	2.23	0.54
2:B:2013:ARG:HE	2:B:2078:GLU:HG2	1.73	0.54
1:A:275:LEU:HD11	1:A:283:LEU:HD22	1.89	0.54
2:B:2302:LEU:HD12	2:B:2302:LEU:N	2.21	0.54
2:B:1056:GLU:O	2:B:1060:LYS:HG2	2.08	0.54
1:A:282:ILE:HD11	2:B:1640:THR:HB	1.89	0.54
2:B:2028:SER:O	2:B:2030:PRO:HD3	2.09	0.53
2:B:1711:VAL:HG12	2:B:1791:PHE:HB3	1.90	0.53
1:A:153:LEU:HD12	1:A:157:LEU:HD13	1.91	0.52
2:B:2259:ILE:HD11	2:B:2293:ILE:HD11	1.91	0.52
2:B:1669:LEU:HD22	2:B:1703:MET:CE	2.40	0.52
2:B:2163:TYR:CE2	2:B:2164:LEU:HD23	2.45	0.52
1:A:50:ASP:O	1:A:52:SER:N	2.41	0.52
2:B:1382:ARG:NH1	3:B:3013:HOH:O	2.43	0.51
2:B:1624:LEU:C	2:B:1624:LEU:HD23	2.31	0.51
1:A:276:PRO:HG2	1:A:279:TYR:CD2	2.46	0.51
2:B:1500:HIS:NE2	2:B:2267:LYS:HE2	2.25	0.51
2:B:1273:GLN:HG2	3:B:2670:HOH:O	2.10	0.50
2:B:1854:ASP:OD1	2:B:1937:ARG:CD	2.59	0.50
1:A:12:GLU:HG3	1:A:25:LYS:HA	1.93	0.50
1:A:16:GLY:HA3	1:A:45:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1867:GLU:N	2:B:1867:GLU:CD	2.64	0.50
2:B:1669:LEU:HD22	2:B:1703:MET:HE3	1.93	0.50
2:B:1704:GLU:HG2	3:B:2570:HOH:O	2.11	0.50
2:B:2152:TRP:CZ3	2:B:2388:ARG:HD3	2.47	0.50
1:A:50:ASP:C	1:A:52:SER:H	2.15	0.50
2:B:1795:LYS:HB3	2:B:1796:PRO:HD3	1.94	0.50
2:B:1605:ARG:NE	2:B:1824:GLN:OE1	2.43	0.50
2:B:902:PRO:O	2:B:955:LYS:NZ	2.44	0.49
2:B:2077:THR:O	2:B:2078:GLU:CG	2.60	0.49
2:B:2395:PHE:O	2:B:2396:SER:C	2.50	0.49
2:B:1960:GLU:HA	2:B:1960:GLU:OE1	2.11	0.49
2:B:1570:TRP:CZ2	2:B:1572:GLY:HA2	2.47	0.49
2:B:1942:ASP:HB2	2:B:1943:PRO:HD3	1.94	0.49
2:B:909:THR:HG23	2:B:910:LYS:N	2.27	0.49
2:B:1104:ILE:HG22	2:B:1107:LEU:HD13	1.94	0.49
2:B:1140:ASN:OD1	2:B:1148:LYS:NZ	2.28	0.49
2:B:1378:LYS:O	2:B:1379:MET:HB3	2.13	0.48
2:B:1651:ALA:HB3	3:B:2621:HOH:O	2.12	0.48
2:B:2354:GLY:O	2:B:2355:ASN:HB2	2.14	0.48
1:A:53:SER:O	2:B:1642:LYS:NZ	2.46	0.48
2:B:1286:TRP:CE2	2:B:1302:LEU:HD11	2.48	0.48
2:B:1104:ILE:CG2	2:B:1107:LEU:HD13	2.43	0.48
1:A:3:THR:HG22	1:A:5:PRO:HD3	1.95	0.48
2:B:2024:MET:SD	2:B:2157:ILE:HG22	2.53	0.48
2:B:2183:TYR:CE2	2:B:2219:LYS:HD3	2.49	0.47
2:B:1666:CYS:SG	2:B:1683:LYS:HE3	2.55	0.47
2:B:2309:ASP:O	2:B:2313:GLN:HG2	2.15	0.47
1:A:344:PRO:HB3	2:B:1858:TYR:CE2	2.50	0.47
2:B:1503:ALA:O	2:B:1506:ARG:NH1	2.45	0.47
2:B:2063:TYR:CD1	2:B:2063:TYR:C	2.87	0.47
1:A:320:ASP:N	1:A:320:ASP:OD1	2.47	0.47
2:B:920:LYS:O	2:B:921:ASP:C	2.53	0.47
2:B:1867:GLU:CD	2:B:1867:GLU:H	2.18	0.47
1:A:86:GLY:O	1:A:90:GLU:HG3	2.15	0.47
2:B:2177:VAL:CG2	2:B:2180:GLN:HB2	2.44	0.47
2:B:2189:LEU:HD11	2:B:2347:GLY:HA3	1.97	0.47
2:B:2228:PRO:HD3	2:B:2352:PRO:HG3	1.97	0.46
2:B:1091:ASN:OD1	2:B:1096:SER:CB	2.57	0.46
2:B:2019:GLU:CG	2:B:2023:LYS:HD2	2.45	0.46
1:A:194:GLU:OE1	3:A:506:HOH:O	2.20	0.46
2:B:996:ASP:OD2	2:B:1511:ARG:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1005:GLN:OE1	2:B:1506:ARG:NH2	2.49	0.46
2:B:1687:HIS:CD2	2:B:1688:PRO:CD	2.98	0.46
2:B:920:LYS:HG3	2:B:940:ILE:HG21	1.96	0.46
2:B:1021:PRO:HB2	2:B:1022:PRO:HD3	1.98	0.46
2:B:958:LEU:HA	2:B:1081:TYR:CD2	2.50	0.46
2:B:988:GLU:O	2:B:991:THR:CG2	2.63	0.46
2:B:1706:VAL:HG12	2:B:1707:HIS:N	2.31	0.46
2:B:2060:LEU:HA	2:B:2063:TYR:HB3	1.98	0.46
2:B:1035:LEU:CD1	2:B:1171:LEU:CD2	2.94	0.45
2:B:1286:TRP:HB2	2:B:1300:ALA:HB3	1.97	0.45
2:B:1739:ARG:HD3	3:B:2501:HOH:O	2.15	0.45
1:A:16:GLY:O	1:A:44:ILE:HA	2.17	0.45
2:B:1673:LEU:HA	2:B:1678:ILE:HB	1.99	0.45
2:B:1639:PRO:C	2:B:1640:THR:HG23	2.36	0.45
1:A:150:ASN:ND2	1:A:175:SER:OG	2.49	0.45
2:B:2177:VAL:HG23	2:B:2180:GLN:HB2	1.98	0.45
2:B:2223:THR:HG21	2:B:2350:ILE:CG1	2.47	0.45
2:B:920:LYS:O	2:B:922:VAL:N	2.51	0.44
1:A:54:MET:SD	1:A:143:SER:HB3	2.57	0.44
2:B:1720:THR:HA	3:B:2897:HOH:O	2.18	0.44
1:A:83:GLU:CG	1:A:89:PHE:HB2	2.48	0.44
2:B:988:GLU:OE1	3:B:2695:HOH:O	2.21	0.44
2:B:1092:PHE:HE1	2:B:1093:LYS:HE3	1.82	0.44
2:B:2149:LYS:HZ3	2:B:2149:LYS:HA	1.83	0.44
2:B:930:ASN:CG	2:B:931:ALA:N	2.71	0.44
2:B:1840:TYR:HH	2:B:2005:PHE:HD2	1.63	0.44
1:A:134:GLU:OE1	1:A:134:GLU:N	2.34	0.44
2:B:1366:ARG:HD2	3:B:2885:HOH:O	2.16	0.44
2:B:1904:ARG:HH11	2:B:1904:ARG:HG2	1.83	0.44
2:B:909:THR:HG23	2:B:910:LYS:H	1.81	0.44
2:B:1035:LEU:HB2	2:B:1038:ILE:HB	1.99	0.44
2:B:1036:SER:OG	2:B:1154:LYS:CE	2.66	0.44
2:B:1272:ARG:O	2:B:1274:ARG:N	2.50	0.44
2:B:1687:HIS:CD2	2:B:1688:PRO:N	2.86	0.44
2:B:2165:ARG:O	2:B:2299:SER:HA	2.18	0.43
1:A:355:PRO:CB	2:B:2267:LYS:HD3	2.48	0.43
2:B:1085:LYS:HE2	3:B:2749:HOH:O	2.18	0.43
2:B:1157:PRO:O	2:B:1172:PHE:HA	2.18	0.43
2:B:1077:ASN:ND2	3:B:3010:HOH:O	2.28	0.43
2:B:1708:GLU:O	3:B:2962:HOH:O	2.21	0.43
2:B:1093:LYS:HB3	2:B:1094:ASP:H	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1666:CYS:SG	2:B:1683:LYS:CE	3.06	0.43
2:B:1307:GLU:O	2:B:1311:LYS:HG3	2.18	0.43
2:B:1383:PHE:CE2	2:B:1387:VAL:CG2	2.94	0.43
2:B:1480:LEU:O	2:B:1481:GLU:C	2.56	0.43
2:B:969:ILE:HA	2:B:981:VAL:O	2.18	0.43
1:A:50:ASP:O	1:A:50:ASP:CG	2.56	0.43
2:B:1029:THR:HG22	2:B:1260:PHE:HZ	1.84	0.42
1:A:55:ARG:HD2	1:A:233:PHE:O	2.19	0.42
1:A:271:GLN:O	1:A:274:THR:HG22	2.18	0.42
2:B:2002:TYR:O	2:B:2006:SER:OG	2.38	0.42
2:B:1060:LYS:HB3	2:B:1060:LYS:HE2	1.84	0.42
2:B:1710:GLU:HG2	2:B:1728:ILE:HD13	2.01	0.42
2:B:1836:ASN:O	2:B:1840:TYR:N	2.53	0.42
2:B:1851:PHE:O	2:B:1881:THR:HA	2.20	0.42
2:B:1236:THR:O	2:B:1236:THR:HG22	2.20	0.42
2:B:1411:ASP:O	2:B:1559:HIS:HE1	2.01	0.42
2:B:1805:ILE:HD13	2:B:1805:ILE:N	2.34	0.42
2:B:2033:THR:OG1	3:B:2979:HOH:O	2.22	0.42
2:B:1844:PHE:CE1	2:B:2002:TYR:HA	2.54	0.42
2:B:1859:ARG:HD2	2:B:1877:GLY:HA2	2.01	0.42
2:B:1040:ASP:OD2	2:B:1045:GLN:NE2	2.48	0.42
2:B:1073:ILE:HD13	2:B:1116:TYR:CE1	2.54	0.42
2:B:988:GLU:O	2:B:991:THR:HG23	2.20	0.42
2:B:1601:ILE:HG23	2:B:1605:ARG:HD2	2.01	0.42
2:B:1354:GLU:N	2:B:1355:PRO:CD	2.83	0.42
1:A:85:ASP:HB3	1:A:88:LYS:HB3	2.02	0.41
2:B:1512:ARG:HG3	3:B:2868:HOH:O	2.19	0.41
2:B:2238:ILE:HG22	2:B:2239:SER:O	2.20	0.41
2:B:1624:LEU:HD21	2:B:1633:PHE:CD1	2.55	0.41
1:A:120:PHE:CE2	1:A:263:LYS:HE3	2.55	0.41
2:B:1001:TYR:HA	2:B:1506:ARG:HG3	2.02	0.41
2:B:1285:VAL:HG12	2:B:1301:TYR:CD2	2.56	0.41
2:B:2157:ILE:CD1	3:B:2943:HOH:O	2.68	0.41
2:B:1092:PHE:CE1	2:B:1093:LYS:HG3	2.56	0.41
2:B:1194:ASN:HB2	2:B:1196:GLU:HG3	2.03	0.41
2:B:1784:TYR:CD1	2:B:1806:MET:HG3	2.55	0.41
1:A:275:LEU:CD1	1:A:283:LEU:HD22	2.49	0.41
2:B:1611:SER:N	2:B:1612:PRO:CD	2.84	0.41
2:B:1933:ILE:HG21	2:B:1944:LEU:HD21	2.03	0.41
1:A:167:LYS:O	1:A:168:ASN:C	2.59	0.41
2:B:1162:THR:HG22	2:B:1169:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1440:ILE:HD11	2:B:1539:LEU:HD21	2.02	0.41
2:B:2029:ASP:HB3	2:B:2032:ILE:HD12	2.03	0.41
2:B:2157:ILE:HD13	3:B:2943:HOH:O	2.21	0.41
2:B:1893:ILE:HD12	2:B:1978:VAL:HG22	2.03	0.41
1:A:105:TYR:CD1	1:A:106:PRO:CD	3.03	0.40
2:B:1289:VAL:HG22	2:B:1296:ARG:HH11	1.86	0.40
2:B:1378:LYS:O	2:B:1379:MET:CB	2.69	0.40
2:B:2177:VAL:HG23	2:B:2177:VAL:O	2.20	0.40
2:B:2279:LYS:HE2	3:B:2931:HOH:O	2.22	0.40
2:B:1376:ASN:HB3	3:B:3014:HOH:O	2.21	0.40
2:B:1710:GLU:HG2	2:B:1728:ILE:CD1	2.51	0.40
2:B:1742:ASP:OD1	2:B:1742:ASP:C	2.60	0.40
1:A:58:TYR:HA	1:A:138:SER:O	2.22	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)
3:B:2720:HOH:O	3:B:2814:HOH:O[3_655]	2.10	0.10

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	324/384 (84%)	306 (94%)	16 (5%)	2 (1%)	25 19
2	B	1393/1564 (89%)	1336 (96%)	50 (4%)	7 (0%)	29 23
All	All	1717/1948 (88%)	1642 (96%)	66 (4%)	9 (0%)	29 23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	320	ASP
2	B	921	ASP
2	B	1376	ASN
2	B	883	SER
2	B	2384	ASN
2	B	1379	MET
2	B	1845	ASN
2	B	947	PRO

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	305/348 (88%)	303 (99%)	2 (1%)	84	88
2	B	1265/1397 (91%)	1229 (97%)	36 (3%)	43	44
All	All	1570/1745 (90%)	1532 (98%)	38 (2%)	49	51

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	281	ASP
2	B	883	SER
2	B	894	SER
2	B	930	ASN
2	B	936	GLU
2	B	969	ILE
2	B	991	THR
2	B	1094	ASP
2	B	1095	MET
2	B	1097	HIS
2	B	1275	MET
2	B	1282	ASP
2	B	1288	LEU
2	B	1297	THR

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Mol	Chain	Res	Type
2	B	1323	SER
2	B	1326	THR
2	B	1378	LYS
2	B	1481	GLU
2	B	1506	ARG
2	B	1573	LEU
2	B	1686	VAL
2	B	1762	ASP
2	B	1769	SER
2	B	1805	ILE
2	B	1826	TYR
2	B	1864	LYS
2	B	1867	GLU
2	B	2006	SER
2	B	2031	THR
2	B	2063	TYR
2	B	2072	SER
2	B	2147	SER
2	B	2149	LYS
2	B	2178	GLU
2	B	2296	THR
2	B	2367	ASN
2	B	2388	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	45	HIS
1	A	150	ASN
2	B	1516	GLN
2	B	1559	HIS
2	B	1687	HIS
2	B	2018	ASN
2	B	2070	ASN

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 monosaccharides 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	334/384 (86%)	0.35	23 (6%)	16	16	24, 45, 105, 133	0
2	B	1407/1564 (89%)	0.24	61 (4%)	35	34	23, 49, 85, 127	0
All	All	1741/1948 (89%)	0.26	84 (4%)	30	29	23, 48, 90, 133	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ASN	6.3
2	B	1598	LEU	5.3
1	A	87	ALA	5.1
2	B	2147	SER	5.0
1	A	165	GLU	4.6
1	A	90	GLU	4.6
2	B	2148	SER	4.5
2	B	1092	PHE	4.3
1	A	336	ASP	4.3
2	B	2069	VAL	4.2
1	A	84	ARG	4.2
1	A	38	ILE	4.1
1	A	169	GLU	4.0
2	B	908	ASP	3.9
1	A	167	LYS	3.8
2	B	2068	ASN	3.8
1	A	166	ALA	3.8
2	B	2070	ASN	3.7
1	A	92	ILE	3.7
2	B	2179	GLU	3.7
2	B	1568	ASN	3.6
2	B	2213	LYS	3.6
2	B	2212	ALA	3.6
1	A	157	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	89	PHE	3.5
2	B	2043	PHE	3.5
1	A	338	GLU	3.5
2	B	2064	GLY	3.5
2	B	1484	TRP	3.5
2	B	1763	ASN	3.4
2	B	2057	ASP	3.4
2	B	2063	TYR	3.3
1	A	329	GLY	3.2
2	B	2150	ASN	3.2
2	B	1826	TYR	3.2
1	A	101	MET	3.2
1	A	168	ASN	3.1
2	B	2214	ASP	3.1
2	B	883	SER	3.0
2	B	1323	SER	2.9
2	B	1571	GLU	2.9
1	A	39	GLY	2.9
2	B	1193	PRO	2.7
2	B	2065	ARG	2.7
2	B	2245	GLY	2.7
2	B	1296	ARG	2.7
2	B	2176	PHE	2.5
2	B	2361	PHE	2.5
2	B	1995	TRP	2.5
1	A	88	LYS	2.5
1	A	85	ASP	2.4
2	B	1276	GLU	2.4
2	B	2067	TYR	2.4
2	B	2056	ARG	2.4
2	B	1093	LYS	2.4
2	B	2049	ILE	2.4
2	B	2078	GLU	2.4
2	B	1998	ARG	2.4
2	B	2345	ILE	2.3
2	B	2048	TRP	2.3
2	B	2050	THR	2.3
2	B	1996	LEU	2.3
2	B	1764	VAL	2.3
2	B	1281	ASN	2.3
2	B	1094	ASP	2.2
2	B	1431	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	2216	PRO	2.2
1	A	107	LYS	2.2
2	B	2244	ILE	2.2
2	B	2037	TYR	2.2
2	B	2366	PHE	2.1
2	B	1497	ARG	2.1
2	B	2364	THR	2.1
2	B	2032	ILE	2.1
2	B	1521	ARG	2.1
1	A	104	SER	2.1
2	B	2246	ASP	2.1
2	B	1686	VAL	2.1
2	B	1767	TYR	2.1
2	B	2149	LYS	2.1
1	A	339	ASP	2.1
2	B	1623	PHE	2.1
2	B	1573	LEU	2.0
2	B	2210	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.