



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:53 pm BST

PDB ID : 3FAY
Title : Crystal structure of the GAP-related domain of IQGAP1
Authors : Kurella, V.B.; Richard, J.M.; Parke, C.L.; Bellamy, H.; Worthylake, D.K.
Deposited on : 2008-11-18
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

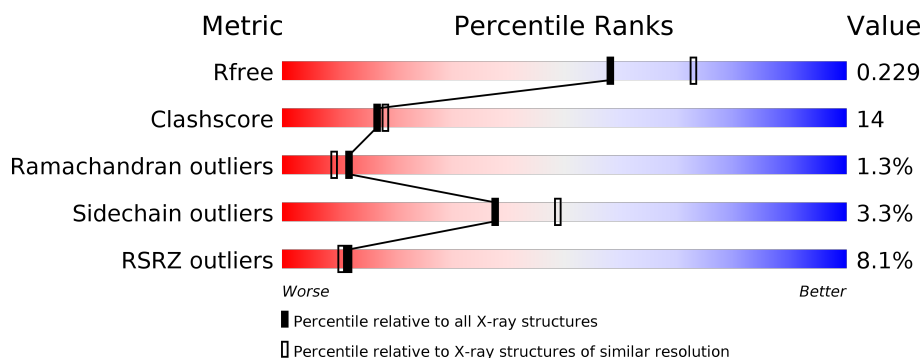
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	<div> <div>8%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3191 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.

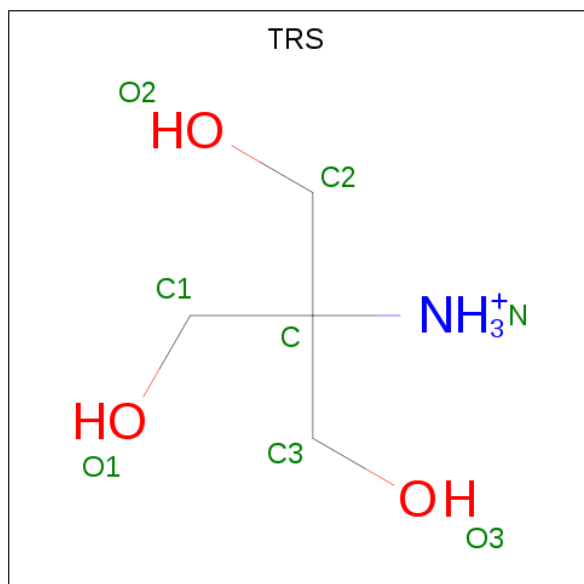
- Molecule 1 is a protein called Ras GTPase-activating-like protein IQGAP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	379	3036	1935	507	583	1	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	SER	-	EXPRESSION TAG	UNP P46940
A	960	ASN	-	EXPRESSION TAG	UNP P46940
A	961	ALA	-	EXPRESSION TAG	UNP P46940

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total 147	O 147	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 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: Ras GTPase-activating-like protein IQGAP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.13Å 42.12Å 59.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 21.27 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.8 (25.00-2.20) 86.9 (21.27-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.258 0.233 , 0.229	Depositor DCC
R_{free} test set	1976 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3191	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.34	0/3083	0.58	1/4158 (0.0%)

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
1	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1283	GLU	N-CA-C	5.77	126.59	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1192	TYR	Sidechain
1	A	1284	TYR	Sidechain

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	A	3036	0	3043	84	0
2	A	8	0	12	2	0
3	A	147	0	0	9	0
All	All	3191	0	3055	86	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 (86) 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:1117:THR:OG1	1:A:1120:GLN:HG2	1.69	0.92
1:A:1337:ILE:H	1:A:1337:ILE:HD12	1.34	0.92
1:A:1041:ILE:HG22	1:A:1042:GLN:H	1.34	0.90
1:A:1116:VAL:HG22	1:A:1120:GLN:HG3	1.55	0.88
1:A:1116:VAL:HA	1:A:1120:GLN:HE21	1.40	0.85
1:A:1250:ILE:HD12	1:A:1250:ILE:H	1.43	0.82
1:A:1290:LEU:H	1:A:1290:LEU:HD23	1.44	0.82
1:A:1017:ARG:HD3	1:A:1290:LEU:HD21	1.63	0.80
1:A:1098:TRP:CZ2	1:A:1126:GLU:HG3	2.19	0.78
1:A:1044:ILE:HD11	1:A:1171:LEU:HD21	1.71	0.73
1:A:1181:ASP:OD1	1:A:1263:ARG:HD2	1.90	0.72
1:A:1117:THR:H	1:A:1120:GLN:NE2	1.88	0.71
1:A:1158:TYR:HE1	1:A:1272:VAL:CG1	2.04	0.70
1:A:1098:TRP:CE2	1:A:1126:GLU:HG3	2.26	0.69
1:A:1158:TYR:CE1	1:A:1272:VAL:CG1	2.75	0.68
1:A:1116:VAL:CA	1:A:1120:GLN:HE21	2.07	0.68
1:A:1116:VAL:HA	1:A:1120:GLN:NE2	2.08	0.67
1:A:1017:ARG:HH11	1:A:1290:LEU:HD11	1.60	0.67
1:A:1247:HIS:CD2	1:A:1248:LEU:HD13	2.31	0.66
1:A:1250:ILE:HD12	1:A:1250:ILE:N	2.10	0.65
2:A:1:TRS:H22	3:A:144:HOH:O	1.97	0.63
1:A:1041:ILE:C	1:A:1043:GLU:H	2.02	0.63
1:A:1189:ASN:HD21	1:A:1194:ARG:HE	1.45	0.62
1:A:1250:ILE:CD1	1:A:1250:ILE:H	2.14	0.61
1:A:1303:ILE:HG12	1:A:1335:PRO:HG2	1.83	0.61
1:A:1017:ARG:NH1	1:A:1290:LEU:HD11	2.16	0.60
1:A:1117:THR:H	1:A:1120:GLN:HE21	1.50	0.58
1:A:1291:THR:HA	3:A:131:HOH:O	2.02	0.58
1:A:1222:ARG:HB2	1:A:1222:ARG:NH1	2.18	0.58
1:A:1152:SER:HB3	1:A:1155:LYS:HD2	1.87	0.56
1:A:1287:LEU:HB2	3:A:78:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:THR:OG1	1:A:1221:GLN:HG3	2.06	0.55
2:A:1:TRS:H31	3:A:144:HOH:O	2.07	0.55
1:A:1158:TYR:CE1	1:A:1272:VAL:HG11	2.42	0.55
1:A:1132:ASP:O	1:A:1136:ARG:HG2	2.06	0.55
1:A:1272:VAL:HG13	1:A:1273:PRO:HD2	1.88	0.55
1:A:1041:ILE:O	1:A:1043:GLU:N	2.36	0.54
1:A:1242:LEU:HD13	3:A:56:HOH:O	2.08	0.54
1:A:1073:ALA:HB3	1:A:1074:PRO:HD3	1.90	0.54
1:A:1117:THR:H	1:A:1120:GLN:CG	2.22	0.53
1:A:990:ILE:HA	1:A:1002:MSE:HE2	1.90	0.53
1:A:1041:ILE:HG22	1:A:1042:GLN:N	2.14	0.52
1:A:1117:THR:N	1:A:1120:GLN:HE21	2.07	0.51
1:A:1182:GLU:O	1:A:1186:ILE:HG12	2.09	0.51
1:A:1076:VAL:O	1:A:1080:MSE:HG2	2.10	0.51
1:A:1033:GLU:O	1:A:1037:LYS:HB2	2.11	0.51
1:A:1049:PRO:HG2	1:A:1052:ILE:HB	1.93	0.50
1:A:1126:GLU:O	1:A:1130:ARG:HG3	2.11	0.50
1:A:1079:ILE:HD11	1:A:1141:VAL:HG13	1.94	0.50
1:A:1126:GLU:CD	1:A:1126:GLU:H	2.14	0.50
1:A:1138:MSE:HE1	1:A:1227:SER:HB3	1.94	0.49
1:A:1259:TYR:CZ	1:A:1263:ARG:HG3	2.47	0.49
1:A:1027:LYS:HD2	1:A:1162:PHE:HZ	1.78	0.48
1:A:1189:ASN:ND2	1:A:1194:ARG:HE	2.12	0.48
1:A:1238:ASN:HB2	1:A:1259:TYR:CG	2.48	0.48
1:A:1017:ARG:CD	1:A:1290:LEU:HD21	2.41	0.48
1:A:1095:TYR:O	1:A:1098:TRP:HB3	2.15	0.47
1:A:984:THR:CG2	1:A:988:LYS:HZ2	2.28	0.47
1:A:1089:THR:HG21	3:A:77:HOH:O	2.14	0.47
1:A:963:LYS:O	1:A:967:GLU:HG3	2.15	0.47
1:A:1041:ILE:C	1:A:1043:GLU:N	2.69	0.46
1:A:1141:VAL:HG11	1:A:1228:ILE:HD11	1.97	0.46
1:A:1279:PHE:O	1:A:1281:VAL:HG13	2.16	0.46
1:A:1327:LEU:O	1:A:1331:LEU:HB2	2.16	0.46
1:A:1095:TYR:CD2	1:A:1116:VAL:HG11	2.51	0.45
1:A:1286:ASP:O	1:A:1287:LEU:HB2	2.16	0.45
1:A:1284:TYR:C	1:A:1286:ASP:N	2.68	0.44
1:A:1088:LYS:O	1:A:1134:SER:HB3	2.18	0.43
1:A:1222:ARG:HD3	3:A:120:HOH:O	2.17	0.43
1:A:1299:ILE:HG12	3:A:47:HOH:O	2.17	0.43
1:A:1281:VAL:HG11	1:A:1287:LEU:HG	2.01	0.43
1:A:1040:GLN:HA	1:A:1175:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:LEU:HD11	1:A:1217:LEU:HD12	2.00	0.42
1:A:999:THR:HG21	1:A:1053:LYS:HG3	2.00	0.42
1:A:1283:GLU:O	1:A:1284:TYR:CB	2.68	0.42
1:A:1117:THR:H	1:A:1120:GLN:CD	2.22	0.42
1:A:1222:ARG:HB2	1:A:1222:ARG:HH11	1.84	0.41
1:A:1291:THR:HB	3:A:123:HOH:O	2.19	0.41
1:A:1065:GLN:NE2	1:A:1207:ASP:HB2	2.35	0.41
1:A:1119:GLU:HG3	1:A:1120:GLN:N	2.36	0.41
1:A:1002:MSE:O	1:A:1006:ILE:HG12	2.21	0.41
1:A:1303:ILE:CG1	1:A:1335:PRO:HG2	2.51	0.41
1:A:1272:VAL:HG13	1:A:1273:PRO:CD	2.51	0.41
1:A:1336:THR:C	1:A:1338:GLU:N	2.75	0.40
1:A:963:LYS:HG2	1:A:967:GLU:OE2	2.22	0.40
1:A:972:TYR:OH	1:A:1306:HIS:CD2	2.75	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
1	A	377/387 (97%)	353 (94%)	19 (5%)	5 (1%)	12 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1041	ILE
1	A	1284	TYR
1	A	1042	GLN
1	A	1082	ASP
1	A	1288	VAL

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
1	A	338/337 (100%)	327 (97%)	11 (3%)	38 49

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	966	ARG
1	A	1017	ARG
1	A	1030	LEU
1	A	1053	LYS
1	A	1136	ARG
1	A	1177	ASP
1	A	1216	GLN
1	A	1248	LEU
1	A	1262	PHE
1	A	1290	LEU
1	A	1338	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1031	GLN
1	A	1065	GLN
1	A	1070	GLN
1	A	1120	GLN
1	A	1189	ASN
1	A	1216	GLN
1	A	1224	ASN
1	A	1276	GLN
1	A	1306	HIS
1	A	1313	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

1 ligand is 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	$\# Z > 2$
2	TRS	A	1	-	7,7,7	0.39	0	9,9,9	0.58	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
2	TRS	A	1	-	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	TRS	C2-C-C1-O1
2	A	1	TRS	C3-C-C1-O1
2	A	1	TRS	N-C-C1-O1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	TRS	2	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

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	A	369/387 (95%)	0.34	30 (8%) 12 10	21, 38, 100, 138	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1289	THR	17.2
1	A	1290	LEU	9.6
1	A	1285	SER	8.8
1	A	1213	ALA	8.2
1	A	1288	VAL	5.9
1	A	1284	TYR	5.3
1	A	1040	GLN	5.2
1	A	961	ALA	5.0
1	A	1212	SER	4.8
1	A	1287	LEU	4.3
1	A	1337	ILE	3.7
1	A	997	LYS	3.4
1	A	1109	ALA	3.2
1	A	1177	ASP	3.2
1	A	1283	GLU	3.2
1	A	1286	ASP	3.0
1	A	962	SER	3.0
1	A	1338	GLU	2.8
1	A	1083	LYS	2.8
1	A	964	GLU	2.7
1	A	1336	THR	2.6
1	A	1214	GLY	2.3
1	A	1009	LEU	2.3
1	A	994	PRO	2.3
1	A	1047	GLY	2.3
1	A	1111	LYS	2.2
1	A	1276	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	995	GLN	2.0
1	A	1291	THR	2.0
1	A	963	LYS	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 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TRS	A	1	8/8	0.82	0.20	49,52,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.