Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 05:54 AM EDT

PDB ID	:	3P1J
Title	:	Crystal structure of human GTPase IMAP family member 2 in the nucleotide-free state
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Deposited on	:	2010-09-30
Resolution	:	2.58 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:

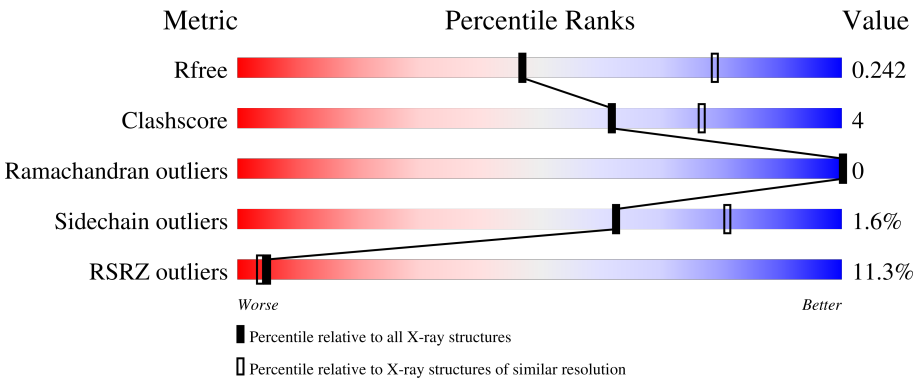
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	209	8% 82% 8% 9%
1	B	209	17% 73% 13% 14%
1	C	209	9% 79% 10% 11%
1	D	209	7% 84% 8% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	D	17	-	-	-	X
2	UNX	D	6	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5399 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 GTPase IMAP family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	190	1392	880	238	262	12	0	0	0
1	B	180	1286	809	224	242	11	0	0	0
1	C	186	1314	828	227	248	11	0	0	0
1	D	193	1388	878	242	258	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q9UG22
B	18	GLY	-	expression tag	UNP Q9UG22
C	18	GLY	-	expression tag	UNP Q9UG22
D	18	GLY	-	expression tag	UNP Q9UG22

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

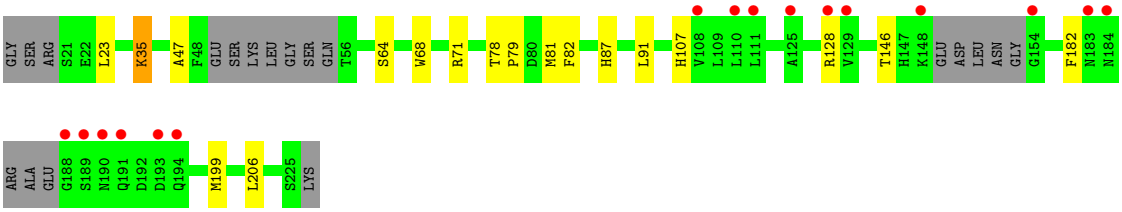
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
2	A	6	6	6	0	0
2	B	4	4	4	0	0
2	C	1	1	1	0	0
2	D	8	8	8	0	0

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.

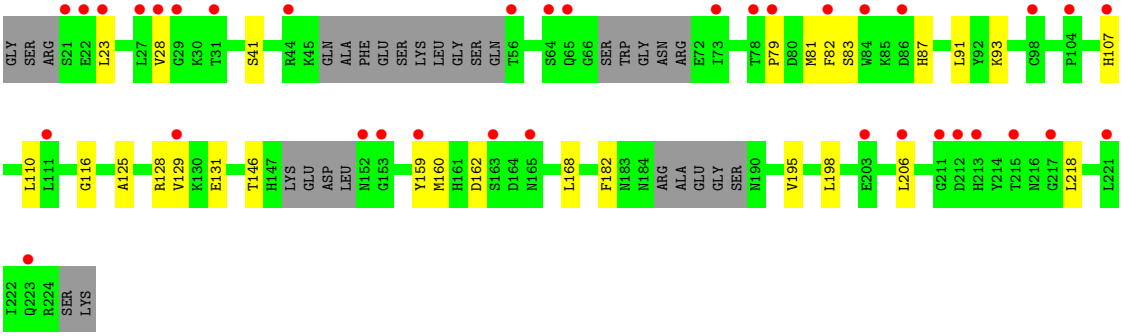
• Molecule 1: GTPase IMAP family member 2

Chain A:



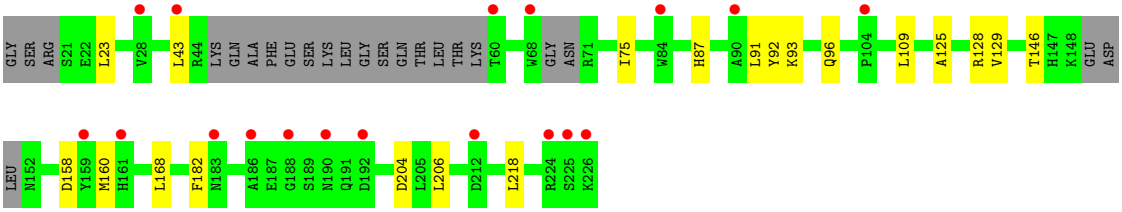
• Molecule 1: GTPase IMAP family member 2

Chain B:



• Molecule 1: GTPase IMAP family member 2

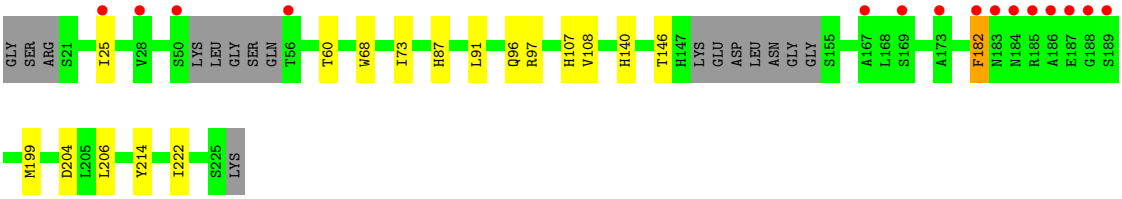
Chain C:



• Molecule 1: GTPase IMAP family member 2

Chain D:

7%
84%
8%
8%


GLY SER ARG S21 I25 V28 S50 LYS LEU GLY SER GLN T56 T60 W68 I73 H87 L91 Q96 R97 H107 V108 H140 T146 H147 LYS GLU ASP LEU ASN GLY GLY S155 A167 L168 S169 A173 F182 N183 N184 R185 A186 E187 G188 S189
M199 D204 L205 L206 Y214 I222 S225 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	132.47Å 132.47Å 84.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.58 29.76 – 2.58	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.58) 100.0 (29.76-2.58)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.57Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.205 , 0.230 0.216 , 0.242	Depositor DCC
R_{free} test set	1005 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5399	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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)

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

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	0.51	0/1411	0.64	0/1907
1	B	0.48	0/1302	0.62	0/1762
1	C	0.49	0/1333	0.60	0/1810
1	D	0.49	0/1407	0.63	0/1907
All	All	0.49	0/5453	0.62	0/7386

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	1392	0	1298	10	0
1	B	1286	0	1157	17	0
1	C	1314	0	1162	12	0
1	D	1388	0	1281	10	0
2	A	6	0	0	0	0
2	B	4	0	0	0	0
2	C	1	0	0	0	0
2	D	8	0	0	0	0
All	All	5399	0	4898	45	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 4.

All (45) 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:C:91:LEU:HD21	1:C:128:ARG:HH12	1.48	0.77
1:A:23:LEU:HD13	1:A:206:LEU:HD11	1.75	0.69
1:B:23:LEU:HD13	1:B:206:LEU:HD11	1.76	0.67
1:B:91:LEU:HD21	1:B:128:ARG:HH22	1.69	0.57
1:D:25:ILE:HG12	1:D:108:VAL:HG13	1.87	0.57
1:B:218:LEU:HD13	1:C:93:LYS:HA	1.88	0.56
1:C:87:HIS:CD2	1:C:91:LEU:HD23	2.41	0.56
1:D:96:GLN:OE1	1:D:222:ILE:HD11	2.08	0.54
1:B:82:PHE:O	1:B:128:ARG:HG3	2.09	0.53
1:B:93:LYS:HA	1:C:218:LEU:HD13	1.90	0.53
1:D:87:HIS:CD2	1:D:91:LEU:HD23	2.44	0.52
1:A:35:LYS:NZ	1:A:78:THR:O	2.42	0.52
1:A:87:HIS:CD2	1:A:91:LEU:HD23	2.44	0.52
1:C:43:LEU:HG	1:C:75:ILE:HD12	1.91	0.52
1:A:146:THR:HA	1:A:182:PHE:O	2.10	0.51
1:B:87:HIS:CD2	1:B:91:LEU:HD23	2.45	0.51
1:A:91:LEU:HD21	1:A:128:ARG:HH22	1.76	0.50
1:D:60:THR:HB	1:D:97:ARG:NH1	2.27	0.50
1:B:28:VAL:HG21	1:B:129:VAL:HG21	1.94	0.50
1:A:82:PHE:O	1:A:128:ARG:HG3	2.13	0.49
1:B:218:LEU:HD11	1:C:96:GLN:CB	2.42	0.49
1:C:23:LEU:HD13	1:C:206:LEU:HD11	1.94	0.48
1:C:125:ALA:O	1:C:129:VAL:HG23	2.14	0.47
1:A:107:HIS:HB3	1:A:206:LEU:HD21	1.96	0.47
1:B:107:HIS:HB3	1:B:206:LEU:HD21	1.96	0.47
1:C:146:THR:HA	1:C:182:PHE:O	2.15	0.47
1:D:68:TRP:HB3	1:D:73:ILE:HD11	1.97	0.46
1:C:91:LEU:HD21	1:C:128:ARG:NH1	2.23	0.46
1:D:68:TRP:CD1	1:D:199:MET:HG3	2.50	0.46
1:D:60:THR:HB	1:D:97:ARG:HH12	1.80	0.45
1:B:160:MET:HE1	1:B:168:LEU:HD21	1.97	0.45
1:B:146:THR:HA	1:B:182:PHE:O	2.17	0.45
1:B:131:GLU:HB3	1:C:92:TYR:HE2	1.81	0.44
1:A:68:TRP:CD1	1:A:199:MET:HG3	2.53	0.44
1:B:79:PRO:HB2	1:B:81:MET:HG2	1.99	0.44
1:B:110:LEU:HD21	1:B:198:LEU:HD11	1.99	0.44
1:B:41:SER:HB3	1:B:195:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:MET:HE1	1:C:168:LEU:HD21	2.01	0.42
1:D:140:HIS:CG	1:D:214:TYR:HB2	2.56	0.41
1:A:47:ALA:HB1	1:A:64:SER:CB	2.51	0.41
1:A:79:PRO:HB2	1:A:81:MET:HG2	2.03	0.41
1:B:83:SER:HB2	1:B:125:ALA:HB2	2.02	0.41
1:B:116:GLY:HA2	1:B:159:TYR:CE2	2.56	0.40
1:D:146:THR:HA	1:D:182:PHE:O	2.21	0.40
1:D:107:HIS:HB3	1:D:206:LEU:HD21	2.04	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	182/209 (87%)	181 (100%)	1 (0%)	0	100	100
1	B	170/209 (81%)	168 (99%)	2 (1%)	0	100	100
1	C	178/209 (85%)	176 (99%)	2 (1%)	0	100	100
1	D	187/209 (90%)	185 (99%)	2 (1%)	0	100	100
All	All	717/836 (86%)	710 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	133/177 (75%)	131 (98%)	2 (2%)	65	82
1	B	116/177 (66%)	115 (99%)	1 (1%)	78	90
1	C	116/177 (66%)	113 (97%)	3 (3%)	46	69
1	D	126/177 (71%)	124 (98%)	2 (2%)	62	81
All	All	491/708 (69%)	483 (98%)	8 (2%)	62	81

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

Mol	Chain	Res	Type
1	A	35	LYS
1	A	71	ARG
1	B	162	ASP
1	C	109	LEU
1	C	158	ASP
1	C	204	ASP
1	D	182	PHE
1	D	204	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 19 ligands modelled in this entry, 19 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	190/209 (90%)	0.29	16 (8%)	11	9	41, 59, 88, 109	0
1	B	180/209 (86%)	0.80	36 (20%)	1	0	47, 71, 99, 134	0
1	C	186/209 (88%)	0.46	18 (9%)	7	6	49, 77, 109, 132	0
1	D	193/209 (92%)	0.38	15 (7%)	13	10	41, 63, 101, 114	0
All	All	749/836 (89%)	0.48	85 (11%)	5	4	41, 68, 102, 134	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	GLY	6.0
1	D	186	ALA	5.8
1	B	206	LEU	5.1
1	D	188	GLY	4.5
1	A	189	SER	4.4
1	B	29	GLY	4.4
1	C	188	GLY	4.2
1	A	190	ASN	4.2
1	D	185	ARG	4.1
1	B	84	TRP	4.1
1	B	215	THR	4.0
1	D	183	ASN	4.0
1	B	65	GLN	3.9
1	C	90	ALA	3.9
1	B	28	VAL	3.8
1	B	73	ILE	3.8
1	B	21	SER	3.7
1	B	211	GLY	3.6
1	D	173	ALA	3.5
1	A	193	ASP	3.4
1	B	223	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	82	PHE	3.3
1	B	78	THR	3.1
1	C	68	TRP	3.0
1	D	56	THR	3.0
1	B	212	ASP	3.0
1	C	104	PRO	3.0
1	A	125	ALA	3.0
1	B	163	SER	2.9
1	A	191	GLN	2.9
1	D	184	ASN	2.9
1	C	192	ASP	2.9
1	B	56	THR	2.9
1	C	225	SER	2.8
1	B	44	ARG	2.8
1	D	169	SER	2.8
1	C	84	TRP	2.8
1	C	183	ASN	2.8
1	B	165	ASN	2.7
1	B	22	GLU	2.7
1	A	129	VAL	2.7
1	B	129	VAL	2.7
1	C	190	ASN	2.6
1	D	187	GLU	2.6
1	A	194	GLN	2.6
1	B	153	GLY	2.6
1	B	27	LEU	2.6
1	A	154	GLY	2.6
1	C	43	LEU	2.5
1	A	128	ARG	2.5
1	B	86	ASP	2.5
1	A	110	LEU	2.5
1	C	186	ALA	2.5
1	B	159	TYR	2.5
1	B	152	ASN	2.5
1	B	64	SER	2.4
1	B	213	HIS	2.4
1	B	111	LEU	2.4
1	C	224	ARG	2.4
1	D	50	SER	2.4
1	B	79	PRO	2.3
1	B	23	LEU	2.3
1	A	148	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	107	HIS	2.3
1	A	111	LEU	2.3
1	C	28	VAL	2.3
1	A	183	ASN	2.2
1	D	28	VAL	2.2
1	C	226	LYS	2.2
1	B	221	LEU	2.2
1	D	189	SER	2.2
1	B	31	THR	2.1
1	A	108	VAL	2.1
1	D	167	ALA	2.1
1	D	25	ILE	2.1
1	B	104	PRO	2.1
1	C	60	THR	2.1
1	B	203	GLU	2.1
1	C	212	ASP	2.1
1	B	98	CYS	2.1
1	C	161	HIS	2.1
1	C	159	TYR	2.1
1	A	184	ASN	2.0
1	D	182	PHE	2.0
1	B	217	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UNX	A	10	1/1	0.59	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UNX	B	14	1/1	0.66	0.20	30,30,30,30	0
2	UNX	D	17	1/1	0.67	0.53	30,30,30,30	0
2	UNX	D	6	1/1	0.71	0.40	61,61,61,61	0
2	UNX	D	5	1/1	0.78	0.28	46,46,46,46	0
2	UNX	D	7	1/1	0.79	0.34	53,53,53,53	0
2	UNX	A	11	1/1	0.82	0.28	30,30,30,30	0
2	UNX	B	2	1/1	0.83	0.70	51,51,51,51	0
2	UNX	B	15	1/1	0.85	0.48	30,30,30,30	0
2	UNX	A	1	1/1	0.86	0.66	50,50,50,50	0
2	UNX	D	228	1/1	0.86	0.37	30,30,30,30	0
2	UNX	A	12	1/1	0.89	0.57	30,30,30,30	0
2	UNX	A	13	1/1	0.90	0.19	30,30,30,30	0
2	UNX	A	9	1/1	0.94	0.34	30,30,30,30	0
2	UNX	D	8	1/1	0.94	0.44	47,47,47,47	0
2	UNX	D	229	1/1	0.94	0.14	30,30,30,30	0
2	UNX	D	227	1/1	0.97	0.53	30,30,30,30	0
2	UNX	B	3	1/1	0.98	0.87	51,51,51,51	0
2	UNX	C	16	1/1	0.98	0.17	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.