Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:32 PM GMT

PDB ID	:	4UCY
Title	:	X-ray structure and activities of an essential Mononegavirales L- protein domain
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Deposited on	:	2014-12-05
Resolution	:	2.83 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 (1)) were used in the production of this report:

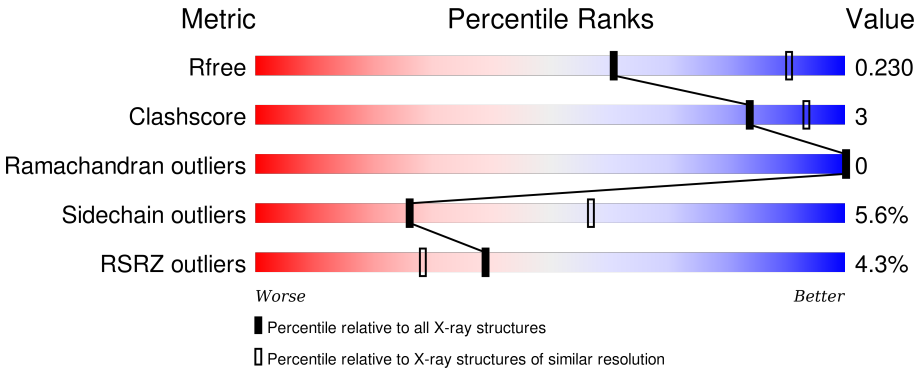
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.83 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}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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	415	6% 82% 12% 6%
1	B	415	2% 79% 12% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6358 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 RNA-DIRECTED RNA POLYMERASE L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3166	2029	542	575	20			
1	B	381	Total	C	N	O	S	0	0	0
			3094	1988	527	559	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1599	MET	-	EXPRESSION TAG	UNP Q91L20
A	2006	SER	-	EXPRESSION TAG	UNP Q91L20
A	2007	GLY	-	EXPRESSION TAG	UNP Q91L20
A	2008	HIS	-	EXPRESSION TAG	UNP Q91L20
A	2009	HIS	-	EXPRESSION TAG	UNP Q91L20
A	2010	HIS	-	EXPRESSION TAG	UNP Q91L20
A	2011	HIS	-	EXPRESSION TAG	UNP Q91L20
A	2012	HIS	-	EXPRESSION TAG	UNP Q91L20
A	2013	HIS	-	EXPRESSION TAG	UNP Q91L20
B	1599	MET	-	EXPRESSION TAG	UNP Q91L20
B	2006	SER	-	EXPRESSION TAG	UNP Q91L20
B	2007	GLY	-	EXPRESSION TAG	UNP Q91L20
B	2008	HIS	-	EXPRESSION TAG	UNP Q91L20
B	2009	HIS	-	EXPRESSION TAG	UNP Q91L20
B	2010	HIS	-	EXPRESSION TAG	UNP Q91L20
B	2011	HIS	-	EXPRESSION TAG	UNP Q91L20
B	2012	HIS	-	EXPRESSION TAG	UNP Q91L20
B	2013	HIS	-	EXPRESSION TAG	UNP Q91L20

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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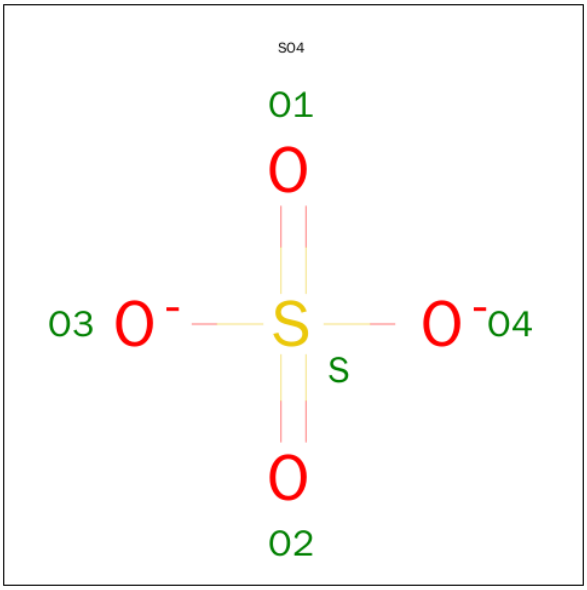
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

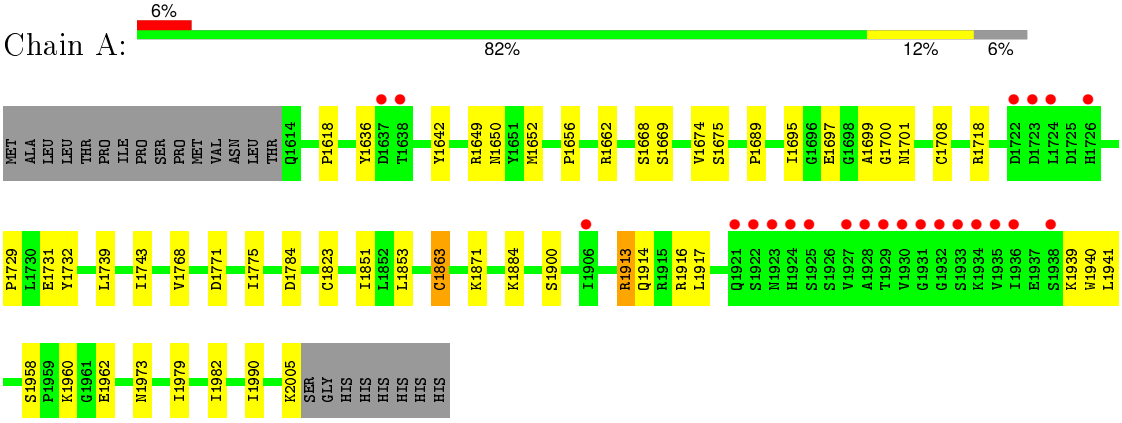
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0
4	B	48	Total O 48 48	0	0

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 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.

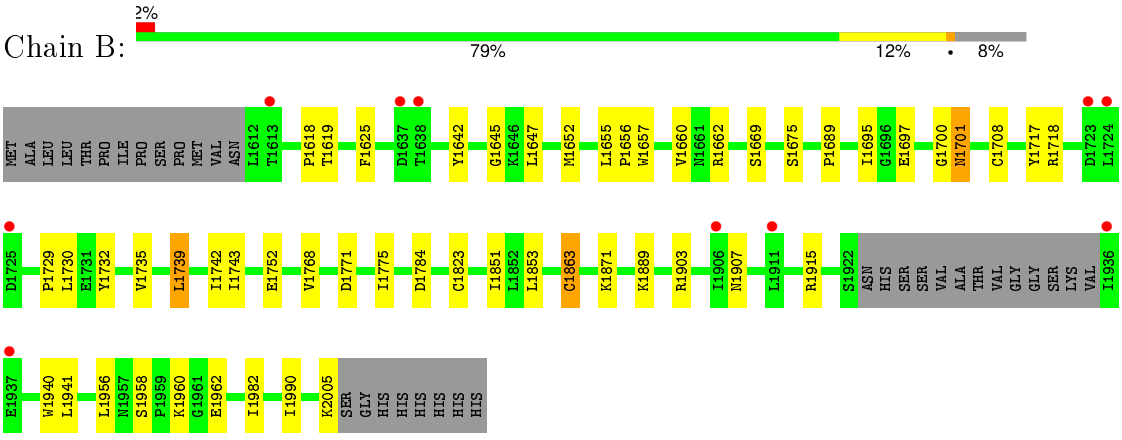
- Molecule 1: RNA-DIRECTED RNA POLYMERASE L

Chain A:



- Molecule 1: RNA-DIRECTED RNA POLYMERASE L

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.23Å 82.16Å 183.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.15 – 2.83 61.15 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.15-2.83) 99.9 (61.15-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.196 , 0.221 0.210 , 0.230	Depositor DCC
R_{free} test set	1378 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	87.7	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.1	EDS
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 28862 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6358	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, SO4

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	0.41	0/3234	0.64	0/4364
1	B	0.40	0/3160	0.63	0/4263
All	All	0.41	0/6394	0.64	0/8627

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

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	3166	0	3206	19	0
1	B	3094	0	3134	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	38	0	0	0	0
4	B	48	0	0	0	0
All	All	6358	0	6340	37	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 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1655:LEU:HD23	1:B:1982:ILE:HD11	1.73	0.71
1:A:1668:SER:HB2	1:A:1699:ALA:HB3	1.71	0.70
1:A:1649:ARG:HD3	1:B:1647:LEU:HB2	1.78	0.62
1:B:1823:CYS:SG	1:B:1863:CYS:HB2	2.41	0.60
1:B:1739:LEU:HG	1:B:1742:ILE:HD12	1.83	0.60
1:B:1851:ILE:HD12	1:B:1853:LEU:HD21	1.83	0.60
1:A:1823:CYS:SG	1:A:1863:CYS:HB2	2.43	0.59
1:B:1618:PRO:HB2	1:B:1708:CYS:HA	1.85	0.58
1:A:1851:ILE:HD12	1:A:1853:LEU:HD21	1.86	0.58
1:A:1656:PRO:HD2	1:A:1990:ILE:HG22	1.85	0.58
1:A:1618:PRO:HB2	1:A:1708:CYS:HA	1.84	0.58
1:A:1960:LYS:HD2	1:A:2005:LYS:HB3	1.87	0.56
1:A:1662:ARG:HD3	1:A:1669:SER:HB2	1.87	0.55
1:B:1960:LYS:HD2	1:B:2005:LYS:HB2	1.90	0.53
1:A:1973:ASN:HB3	1:B:1642:TYR:HB2	1.91	0.52
1:A:1701:ASN:HD22	1:A:1731:GLU:HG2	1.74	0.52
1:B:1662:ARG:HD3	1:B:1669:SER:HB2	1.92	0.51
1:A:1695:ILE:HG22	1:A:1718:ARG:HB2	1.95	0.49
1:B:1697:GLU:HB3	1:B:1717:TYR:CE2	2.47	0.48
1:B:1695:ILE:HG22	1:B:1718:ARG:HB2	1.95	0.48
1:A:1743:ILE:O	1:A:1768:VAL:HG11	2.15	0.47
1:A:1913:ARG:HH12	1:A:1917:LEU:HD22	1.79	0.47
1:B:1729:PRO:HB2	1:B:1732:TYR:HB3	1.97	0.47
1:A:1979:ILE:HD12	1:A:1982:ILE:HD11	1.97	0.46
1:B:1697:GLU:HG3	1:B:1700:GLY:HA2	1.97	0.46
1:A:1689:PRO:HG3	1:A:1775:ILE:HD12	1.98	0.46
1:B:1907:ASN:HA	1:B:1956:LEU:HD11	1.97	0.45
1:B:1656:PRO:HD2	1:B:1990:ILE:HG22	1.99	0.45
1:B:1743:ILE:O	1:B:1768:VAL:HG11	2.16	0.44
1:B:1625:PHE:HE1	1:B:1701:ASN:HD21	1.64	0.44
1:B:1689:PRO:HG3	1:B:1775:ILE:HD12	1.99	0.44
1:B:1657:TRP:O	1:B:1660:VAL:HG22	2.17	0.44
1:A:1697:GLU:HG3	1:A:1700:GLY:HA2	2.01	0.42
1:B:1657:TRP:HE3	1:B:1660:VAL:CG1	2.33	0.42
1:A:1656:PRO:CD	1:A:1990:ILE:HG22	2.50	0.41
1:A:1729:PRO:HB2	1:A:1732:TYR:HB3	2.01	0.41
1:A:1650:ASN:O	1:B:1645:GLY:HA3	2.21	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	390/415 (94%)	376 (96%)	14 (4%)	0	100	100
1	B	377/415 (91%)	367 (97%)	10 (3%)	0	100	100
All	All	767/830 (92%)	743 (97%)	24 (3%)	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	353/374 (94%)	333 (94%)	20 (6%)	25	56
1	B	344/374 (92%)	325 (94%)	19 (6%)	27	58
All	All	697/748 (93%)	658 (94%)	39 (6%)	26	57

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1636	TYR
1	A	1642	TYR
1	A	1652	MET
1	A	1674	VAL
1	A	1675	SER
1	A	1739	LEU
1	A	1771	ASP
1	A	1784	ASP

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Mol	Chain	Res	Type
1	A	1863	CYS
1	A	1871	LYS
1	A	1884	LYS
1	A	1900	SER
1	A	1913	ARG
1	A	1914	GLN
1	A	1916	ARG
1	A	1939	LYS
1	A	1940	TRP
1	A	1941	LEU
1	A	1958	SER
1	A	1962	GLU
1	B	1619	THR
1	B	1652	MET
1	B	1675	SER
1	B	1701	ASN
1	B	1730	LEU
1	B	1735	VAL
1	B	1739	LEU
1	B	1752	GLU
1	B	1771	ASP
1	B	1784	ASP
1	B	1863	CYS
1	B	1871	LYS
1	B	1889	LYS
1	B	1903	ARG
1	B	1915	ARG
1	B	1940	TRP
1	B	1941	LEU
1	B	1958	SER
1	B	1962	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1659	HIS
1	A	1914	GLN
1	A	1984	ASN
1	B	1659	HIS
1	B	1701	ASN
1	B	1984	ASN

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
3	SO4	A	2409	-	4,4,4	0.23	0	6,6,6	0.30	0
3	SO4	B	2409	-	4,4,4	0.22	0	6,6,6	0.14	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
3	SO4	A	2409	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2409	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	392/415 (94%)	0.43	23 (5%)	26	17	65, 88, 160, 197	0
1	B	381/415 (91%)	0.30	10 (2%)	59	49	69, 91, 136, 165	0
All	All	773/830 (93%)	0.36	33 (4%)	39	28	65, 89, 148, 197	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1929	THR	9.3
1	A	1930	VAL	9.2
1	A	1928	ALA	8.1
1	A	1932	GLY	7.3
1	A	1638	THR	7.2
1	A	1933	SER	6.3
1	A	1935	VAL	5.5
1	A	1931	GLY	5.5
1	B	1724	LEU	5.0
1	A	1927	VAL	4.5
1	A	1936	ILE	4.4
1	A	1726	HIS	3.9
1	A	1921	GLN	3.8
1	B	1725	ASP	3.7
1	A	1637	ASP	3.5
1	A	1724	LEU	3.2
1	A	1938	SER	3.0
1	B	1638	THR	3.0
1	B	1911	LEU	2.9
1	A	1934	LYS	2.9
1	B	1723	ASP	2.8
1	A	1923	ASN	2.7
1	A	1723	ASP	2.7
1	B	1936	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1922	SER	2.6
1	A	1924	HIS	2.5
1	B	1613	THR	2.5
1	A	1722	ASP	2.5
1	A	1906	ILE	2.4
1	B	1937	GLU	2.3
1	A	1925	SER	2.2
1	B	1906	ILE	2.1
1	B	1637	ASP	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	2408	1/1	0.99	0.23	0.95	81,81,81,81	0
2	ZN	B	2408	1/1	0.99	0.21	-0.39	89,89,89,89	0
3	SO4	B	2409	5/5	0.98	0.18	-0.63	98,99,99,100	0
3	SO4	A	2409	5/5	0.94	0.17	-0.72	100,101,102,105	0

6.5 Other polymers (i)

There are no such residues in this entry.