



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:11 AM UTC

PDB ID : 4Z7G / pdb_00004z7g
Title : Crystal structure of human IRE1 cytoplasmic kinase-RNase region - apo
Authors : Bayliss, R.; Joshi, A.
Deposited on : 2015-04-07
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

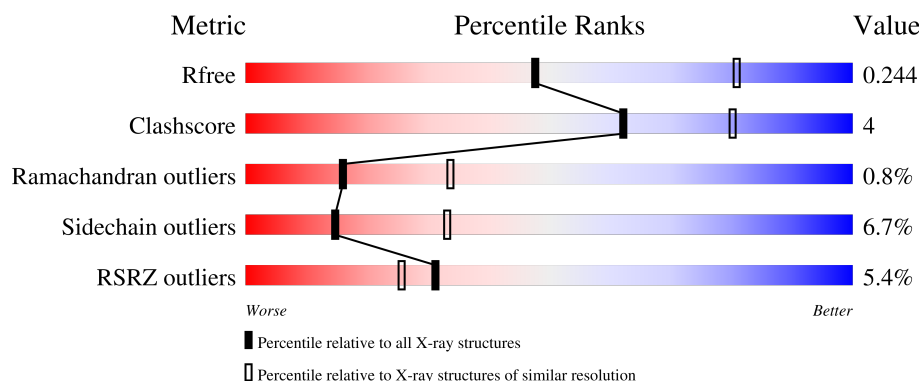
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	416	4% 70% 16% • 12%
1	B	416	5% 75% 13% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6042 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2968	1897	520	533	18			
1	B	377	Total	C	N	O	S	0	0	0
			3057	1955	537	547	18			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

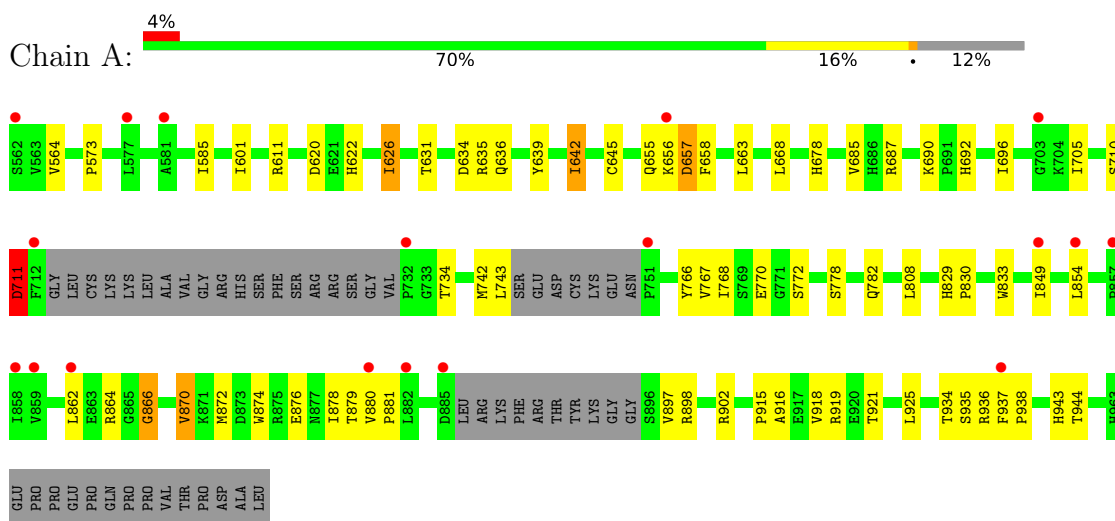
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	7	Total	O	0	0
			7	7		

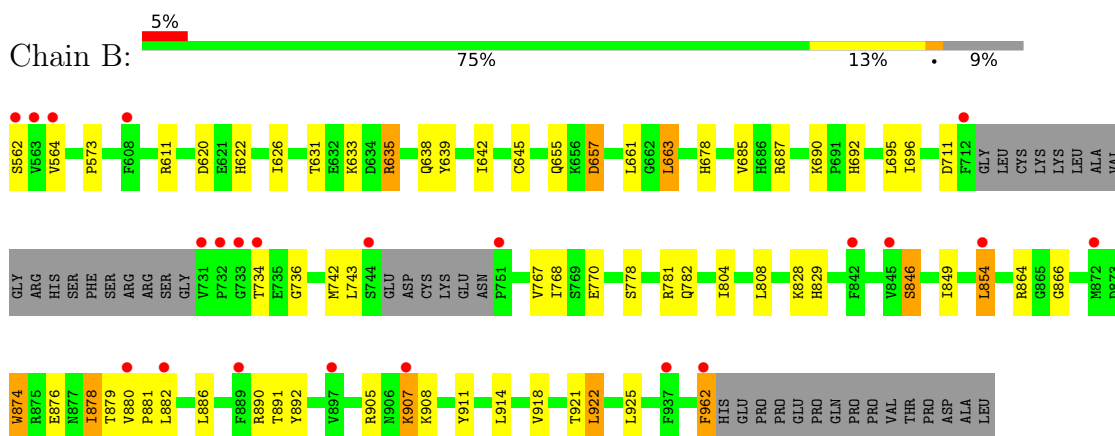
3 Residue-property plots

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: Serine/threonine-protein kinase/endoribonuclease IRE1



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.40Å 78.97Å 86.05Å 90.00° 97.41° 90.00°	Depositor
Resolution (Å)	85.33 – 2.60 85.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (85.33-2.60) 99.5 (85.33-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.203 , 0.226 0.221 , 0.244	Depositor DCC
R_{free} test set	1688 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.7	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	0.95	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: NA

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	0.84	1/3041 (0.0%)	1.44	13/4107 (0.3%)
1	B	0.84	1/3132 (0.0%)	1.42	15/4229 (0.4%)
All	All	0.84	2/6173 (0.0%)	1.43	28/8336 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	880	VAL	CA-CB	5.08	1.56	1.54
1	B	880	VAL	CA-CB	5.02	1.56	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	936	ARG	N-CA-C	-8.25	102.09	112.90
1	A	879	THR	CA-C-N	6.97	127.13	120.43
1	A	879	THR	C-N-CA	6.97	127.13	120.43
1	A	657	ASP	N-CA-C	-6.92	104.02	113.30
1	B	879	THR	CA-C-N	6.91	127.06	120.43
1	B	879	THR	C-N-CA	6.91	127.06	120.43
1	B	866	GLY	CA-C-N	6.44	133.29	121.70
1	B	866	GLY	C-N-CA	6.44	133.29	121.70
1	A	767	VAL	CA-C-N	6.41	128.71	120.70
1	A	767	VAL	C-N-CA	6.41	128.71	120.70
1	B	657	ASP	N-CA-C	-6.23	105.72	113.38
1	A	866	GLY	CA-C-N	6.02	132.53	121.70
1	A	866	GLY	C-N-CA	6.02	132.53	121.70
1	B	890	ARG	CA-C-N	5.79	132.12	121.70
1	B	890	ARG	C-N-CA	5.79	132.12	121.70
1	A	658	PHE	N-CA-C	-5.71	105.98	113.17
1	B	767	VAL	CA-C-N	5.66	127.78	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	767	VAL	C-N-CA	5.66	127.78	120.70
1	B	562	SER	CA-C-N	5.56	131.71	121.70
1	B	562	SER	C-N-CA	5.56	131.71	121.70
1	B	620	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	620	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	897	VAL	CA-C-N	5.45	128.33	120.38
1	A	897	VAL	C-N-CA	5.45	128.33	120.38
1	B	854	LEU	CA-C-N	5.45	131.50	121.70
1	B	854	LEU	C-N-CA	5.45	131.50	121.70
1	A	711	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	657	ASP	CA-CB-CG	5.00	117.60	112.60

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	2968	0	2939	26	0
1	B	3057	0	3040	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0
3	B	7	0	0	0	0
All	All	6042	0	5979	49	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 (49) 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:743:LEU:HD11	1:A:782:GLN:HE21	1.51	0.74
1:A:870:VAL:HG22	1:A:874:TRP:HB3	1.79	0.64
1:B:907:LYS:HE3	1:B:922:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:TYR:HA	1:B:914:LEU:HD12	1.83	0.60
1:B:661:LEU:HB3	1:B:663:LEU:HD13	1.83	0.60
1:A:881:PRO:HG2	1:A:921:THR:HG21	1.84	0.59
1:A:626:ILE:HG12	1:A:710:SER:HB3	1.84	0.59
1:B:846:SER:HB3	1:B:905:ARG:HD3	1.85	0.58
1:B:743:LEU:HD11	1:B:782:GLN:HE21	1.69	0.58
1:B:908:LYS:HG3	1:B:925:LEU:HD11	1.88	0.56
1:B:626:ILE:HD13	1:B:695:LEU:HD12	1.88	0.56
1:B:690:LYS:HD3	1:B:734:THR:OG1	2.09	0.52
1:A:690:LYS:HD3	1:A:734:THR:OG1	2.10	0.52
1:B:828:LYS:HG3	1:B:962:PHE:HB3	1.92	0.52
1:A:663:LEU:HD21	1:A:705:ILE:HB	1.92	0.51
1:B:874:TRP:HD1	1:B:878:ILE:HD12	1.74	0.50
1:A:916:ALA:HA	1:A:919:ARG:HG2	1.94	0.49
1:A:864:ARG:O	1:A:943:HIS:HE1	1.96	0.48
1:A:564:VAL:HG23	1:A:573:PRO:HG3	1.95	0.48
1:A:663:LEU:HD13	1:A:668:LEU:HD21	1.95	0.48
1:A:626:ILE:HD13	1:A:642:ILE:HD11	1.96	0.48
1:B:564:VAL:HG23	1:B:573:PRO:HG3	1.96	0.48
1:A:915:PRO:HG2	1:A:918:VAL:HG22	1.96	0.47
1:A:766:TYR:HA	1:A:772:SER:O	2.14	0.47
1:B:881:PRO:HG2	1:B:921:THR:HG21	1.97	0.46
1:B:882:LEU:HD22	1:B:922:LEU:HD11	1.99	0.45
1:A:685:VAL:HG12	1:A:687:ARG:HG3	2.00	0.44
1:B:685:VAL:HG12	1:B:687:ARG:HG3	1.99	0.44
1:A:622:HIS:HB2	1:A:678:HIS:CD2	2.53	0.44
1:B:622:HIS:HB2	1:B:678:HIS:CD2	2.53	0.43
1:A:690:LYS:HE2	1:A:692:HIS:HB3	1.99	0.43
1:B:633:LYS:HB3	1:B:638:GLN:HG3	2.00	0.43
1:B:690:LYS:HE2	1:B:692:HIS:HB3	2.00	0.43
1:A:874:TRP:HB2	1:A:937:PHE:CZ	2.55	0.42
1:B:736:GLY:HA2	1:B:781:ARG:HB3	2.01	0.42
1:B:645:CYS:HB3	1:B:696:ILE:O	2.19	0.41
1:A:631:THR:HA	1:A:639:TYR:O	2.19	0.41
1:A:626:ILE:HD13	1:A:642:ILE:CG1	2.50	0.41
1:A:849:ILE:HD13	1:A:898:ARG:HG2	2.02	0.41
1:B:808:LEU:HB2	1:B:829:HIS:CE1	2.55	0.41
1:A:830:PRO:HA	1:A:833:TRP:CD2	2.56	0.41
1:B:631:THR:HA	1:B:639:TYR:O	2.21	0.41
1:A:645:CYS:HB3	1:A:696:ILE:O	2.21	0.41
1:A:862:LEU:HD11	1:A:944:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:LEU:HB2	1:A:829:HIS:CE1	2.56	0.40
1:B:635:ARG:NH1	1:B:635:ARG:H	2.19	0.40
1:B:914:LEU:HD22	1:B:918:VAL:HG21	2.04	0.40
1:A:934:THR:HA	1:A:935:SER:HA	1.82	0.40
1:A:935:SER:HB2	1:A:938:PRO:HG3	2.03	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	358/416 (86%)	339 (95%)	16 (4%)	3 (1%)	16	34
1	B	371/416 (89%)	344 (93%)	24 (6%)	3 (1%)	16	34
All	All	729/832 (88%)	683 (94%)	40 (6%)	6 (1%)	16	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ASP
1	B	711	ASP
1	A	770	GLU
1	B	770	GLU
1	B	864	ARG
1	A	866	GLY

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	326/369 (88%)	304 (93%)	22 (7%)	15	33
1	B	335/369 (91%)	313 (93%)	22 (7%)	15	34
All	All	661/738 (90%)	617 (93%)	44 (7%)	15	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	ILE
1	A	601	ILE
1	A	611	ARG
1	A	626	ILE
1	A	634	ASP
1	A	635	ARG
1	A	636	GLN
1	A	642	ILE
1	A	655	GLN
1	A	656	LYS
1	A	657	ASP
1	A	711	ASP
1	A	742	MET
1	A	768	ILE
1	A	778	SER
1	A	854	LEU
1	A	870	VAL
1	A	872	MET
1	A	876	GLU
1	A	878	ILE
1	A	902	ARG
1	A	925	LEU
1	B	611	ARG
1	B	635	ARG
1	B	642	ILE
1	B	655	GLN
1	B	657	ASP
1	B	663	LEU
1	B	742	MET
1	B	768	ILE
1	B	778	SER
1	B	804	ILE
1	B	846	SER

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Mol	Chain	Res	Type
1	B	849	ILE
1	B	854	LEU
1	B	874	TRP
1	B	876	GLU
1	B	878	ILE
1	B	886	LEU
1	B	891	THR
1	B	892	TYR
1	B	907	LYS
1	B	922	LEU
1	B	962	PHE

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	638	GLN
1	A	678	HIS
1	A	702	HIS
1	A	877	ASN
1	A	906	ASN
1	B	579	HIS
1	B	678	HIS
1	B	906	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - 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

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	366/416 (87%)	0.34	18 (4%) 35 29	50, 96, 165, 198	0
1	B	377/416 (90%)	0.35	22 (5%) 29 23	49, 93, 158, 196	0
All	All	743/832 (89%)	0.35	40 (5%) 31 26	49, 94, 161, 198	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	VAL	4.3
1	B	744	SER	3.9
1	A	732	PRO	3.5
1	B	732	PRO	3.4
1	B	937	PHE	3.4
1	A	937	PHE	3.3
1	A	882	LEU	3.2
1	B	751	PRO	3.2
1	A	751	PRO	3.1
1	A	562	SER	3.1
1	B	563	VAL	3.0
1	B	854	LEU	3.0
1	B	562	SER	2.9
1	A	581	ALA	2.9
1	B	897	VAL	2.9
1	A	712	PHE	2.8
1	B	889	PHE	2.7
1	A	857	PRO	2.7
1	B	733	GLY	2.7
1	B	880	VAL	2.7
1	A	854	LEU	2.6
1	B	712	PHE	2.6
1	A	849	ILE	2.6
1	A	577	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	882	LEU	2.5
1	A	880	VAL	2.5
1	B	845	VAL	2.4
1	B	907	LYS	2.4
1	A	862	LEU	2.3
1	B	962	PHE	2.2
1	B	872	MET	2.2
1	A	859	VAL	2.2
1	B	734	THR	2.2
1	A	885	ASP	2.1
1	B	842	PHE	2.1
1	A	703	GLY	2.1
1	A	656	LYS	2.1
1	A	858	ILE	2.1
1	B	608	PHE	2.0
1	B	564	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NA	A	1001	1/1	0.95	0.08	57,57,57,57	0
2	NA	B	1001	1/1	0.97	0.07	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.