Full wwPDB X-ray Structure Validation Report (i)

Nov 9, 2026 – 08:10 PM JST

PDB ID	:	46WF / pdb_000046wf
Title	:	Crystal structure of the Ph-BEACH domains of human LRBA
Authors	:	Collins, B.M.; Eldershaw, D.N.
Deposited on	:	2026-10-13
Resolution	:	1.68 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:

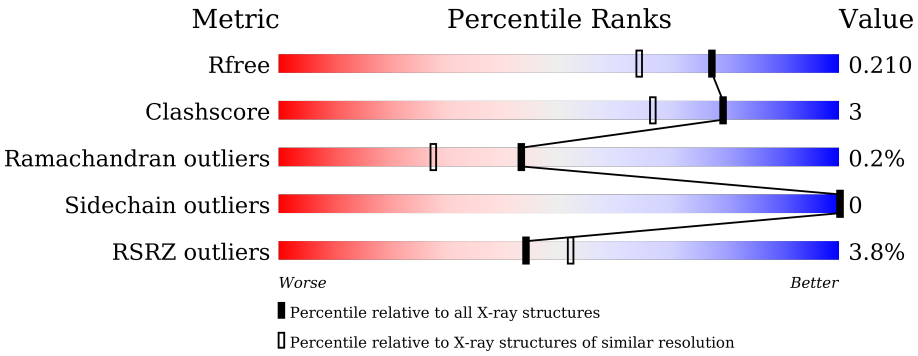
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	438	3% 88% 5% 7%
1	B	438	4% 86% 6% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14698 atoms, of which 7423 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 Lipopolysaccharide-responsive and beige-like anchor protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	H	N	O	S	0	3	0
			6590	2156	3256	554	616	8			
1	B	402	Total	C	H	N	O	S	0	1	0
			6506	2133	3211	547	608	7			

There are 42 discrepancies between the modelled and reference sequences:

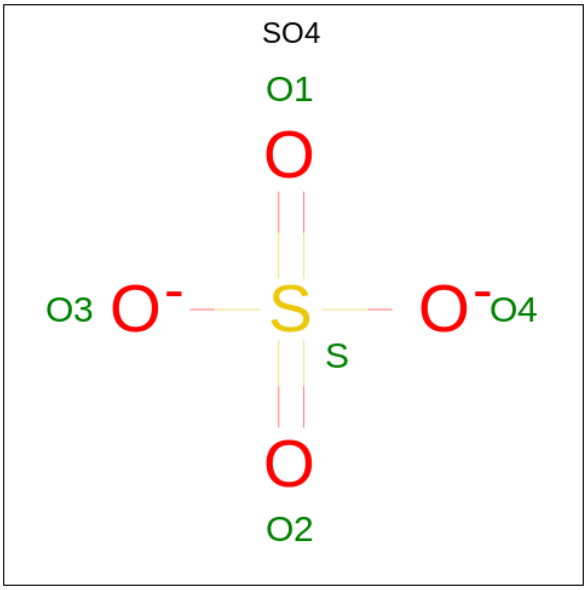
Chain	Residue	Modelled	Actual	Comment	Reference
A	2052	MET	-	initiating methionine	UNP P50851
A	2053	GLY	-	expression tag	UNP P50851
A	2054	SER	-	expression tag	UNP P50851
A	2055	SER	-	expression tag	UNP P50851
A	2056	HIS	-	expression tag	UNP P50851
A	2057	HIS	-	expression tag	UNP P50851
A	2058	HIS	-	expression tag	UNP P50851
A	2059	HIS	-	expression tag	UNP P50851
A	2060	HIS	-	expression tag	UNP P50851
A	2061	HIS	-	expression tag	UNP P50851
A	2062	SER	-	expression tag	UNP P50851
A	2063	SER	-	expression tag	UNP P50851
A	2064	GLY	-	expression tag	UNP P50851
A	2065	LEU	-	expression tag	UNP P50851
A	2066	VAL	-	expression tag	UNP P50851
A	2067	PRO	-	expression tag	UNP P50851
A	2068	ARG	-	expression tag	UNP P50851
A	2069	GLY	-	expression tag	UNP P50851
A	2070	SER	-	expression tag	UNP P50851
A	2071	HIS	-	expression tag	UNP P50851
A	2072	MET	-	expression tag	UNP P50851
B	2052	MET	-	initiating methionine	UNP P50851
B	2053	GLY	-	expression tag	UNP P50851
B	2054	SER	-	expression tag	UNP P50851
B	2055	SER	-	expression tag	UNP P50851

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2056	HIS	-	expression tag	UNP P50851
B	2057	HIS	-	expression tag	UNP P50851
B	2058	HIS	-	expression tag	UNP P50851
B	2059	HIS	-	expression tag	UNP P50851
B	2060	HIS	-	expression tag	UNP P50851
B	2061	HIS	-	expression tag	UNP P50851
B	2062	SER	-	expression tag	UNP P50851
B	2063	SER	-	expression tag	UNP P50851
B	2064	GLY	-	expression tag	UNP P50851
B	2065	LEU	-	expression tag	UNP P50851
B	2066	VAL	-	expression tag	UNP P50851
B	2067	PRO	-	expression tag	UNP P50851
B	2068	ARG	-	expression tag	UNP P50851
B	2069	GLY	-	expression tag	UNP P50851
B	2070	SER	-	expression tag	UNP P50851
B	2071	HIS	-	expression tag	UNP P50851
B	2072	MET	-	expression tag	UNP P50851

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 3 is water.

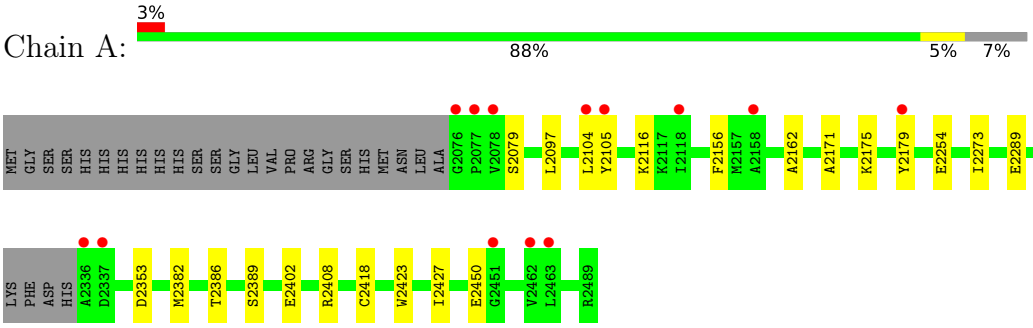
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	361	Total 915	H 554	O 361	0	0
3	B	275	Total 677	H 402	O 275	0	0

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.

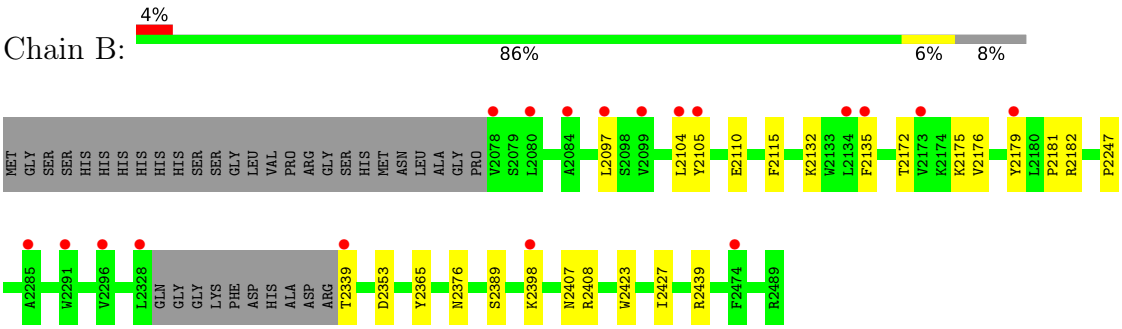
• Molecule 1: Lipopolysaccharide-responsive and beige-like anchor protein

Chain A:



• Molecule 1: Lipopolysaccharide-responsive and beige-like anchor protein

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	75.17Å 75.37Å 171.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 1.68 45.57 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.57-1.68) 99.9 (45.57-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.179 , 0.210 0.179 , 0.210	Depositor DCC
R_{free} test set	2012 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14698	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.86	0/3438	0.84	0/4683
1	B	0.77	0/3392	0.79	1/4621 (0.0%)
All	All	0.81	0/6830	0.81	1/9304 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2398	LYS	CA-CB-CG	-6.06	101.98	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2247	PRO	Peptide

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	3334	3256	3259	19	0
1	B	3295	3211	3218	16	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	361	554	0	8	1
3	B	275	402	0	4	0
All	All	7275	7423	6477	35	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 3.

All (35) 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:2450:GLU:OE2	3:A:2601:HOH:O	2.02	0.77
1:A:2418[A]:CYS:SG	3:A:2943:HOH:O	2.52	0.67
1:B:2376[B]:ASN:OD1	3:B:2601:HOH:O	2.15	0.64
1:A:2175:LYS:N	1:A:2175:LYS:HD3	2.13	0.62
1:A:2289:GLU:CD	3:A:2602:HOH:O	2.42	0.62
1:B:2339:THR:HA	3:B:2790:HOH:O	2.02	0.60
1:A:2382:MET:HE2	1:A:2386:THR:HB	1.84	0.60
1:A:2097:LEU:HD12	1:A:2105:TYR:O	2.02	0.59
1:B:2175:LYS:O	1:B:2179:TYR:HD2	1.86	0.59
1:A:2289:GLU:OE2	3:A:2602:HOH:O	2.17	0.59
1:A:2097:LEU:HD11	1:A:2104:LEU:HD11	1.85	0.58
1:B:2439:ARG:HG2	1:B:2439:ARG:HH11	1.68	0.58
1:A:2097:LEU:HD11	1:A:2104:LEU:CD1	2.37	0.54
1:A:2116:LYS:HE3	1:A:2116:LYS:HA	1.93	0.51
1:A:2254:GLU:OE2	1:A:2254:GLU:HA	2.09	0.51
1:B:2172:THR:O	1:B:2176:VAL:HG23	2.10	0.50
1:B:2097:LEU:HD11	1:B:2104:LEU:HD11	1.93	0.49
1:A:2408:ARG:NH2	3:A:2606:HOH:O	2.45	0.48
1:A:2079:SER:HB3	1:A:2179:TYR:CE2	2.48	0.48
1:A:2402:GLU:CD	3:A:2605:HOH:O	2.57	0.48
1:B:2175:LYS:O	1:B:2179:TYR:CD2	2.65	0.48
1:B:2110:GLU:HG2	1:B:2115:PHE:CZ	2.50	0.47
1:B:2353:ASP:HB2	3:B:2818:HOH:O	2.15	0.45
1:A:2171:ALA:O	1:A:2175:LYS:HG2	2.17	0.44
1:A:2156:PHE:CD2	1:A:2162:ALA:HB2	2.54	0.42
1:B:2105:TYR:CE1	1:B:2132:LYS:HD3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2110:GLU:HG2	1:B:2115:PHE:CE1	2.54	0.42
1:A:2353:ASP:HB2	3:A:2832:HOH:O	2.20	0.42
1:B:2182:ARG:NH1	2:B:2501:SO4:O2	2.53	0.41
1:A:2423:TRP:CZ2	1:A:2427:ILE:HG13	2.55	0.41
1:B:2423:TRP:CZ2	1:B:2427:ILE:HG13	2.56	0.41
1:B:2135:PHE:CD2	1:B:2181:PRO:HD3	2.56	0.41
1:B:2365:TYR:O	1:B:2408:ARG:HD2	2.21	0.41
1:A:2273:ILE:HD12	3:A:2603:HOH:O	2.21	0.40
1:B:2407:ASN:CB	3:B:2616:HOH:O	2.69	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:A:2602:HOH:O	3:A:2605:HOH:O[3_555]	2.18	0.02

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	406/438 (93%)	396 (98%)	9 (2%)	1 (0%)	43	27
1	B	399/438 (91%)	391 (98%)	7 (2%)	1 (0%)	36	21
All	All	805/876 (92%)	787 (98%)	16 (2%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2389	SER
1	B	2389	SER

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	369/391 (94%)	369 (100%)	0	100	100
1	B	364/391 (93%)	364 (100%)	0	100	100
All	All	733/782 (94%)	733 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2085	GLN
1	A	2166	ASN
1	A	2213	GLN
1	A	2242	GLN
1	A	2373	ASN
1	A	2375	ASN
1	A	2433	GLN
1	B	2375	ASN
1	B	2432	GLN
1	B	2433	GLN
1	B	2470	GLN

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)

2 ligands are 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	SO4	A	2501	-	4,4,4	0.42	0	6,6,6	0.43	0
2	SO4	B	2501	-	4,4,4	0.56	0	6,6,6	0.47	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2501	SO4	1	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, 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	407/438 (92%)	0.04	13 (3%) 50 57	15, 34, 67, 79	3 (0%)
1	B	402/438 (91%)	0.39	18 (4%) 38 47	23, 41, 70, 84	1 (0%)
All	All	809/876 (92%)	0.21	31 (3%) 44 52	15, 37, 69, 84	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2078	VAL	4.7
1	B	2328	LEU	3.7
1	A	2336	ALA	3.6
1	B	2179	TYR	3.5
1	A	2104	LEU	3.5
1	A	2076	GLY	3.4
1	B	2296	VAL	3.3
1	B	2080	LEU	2.9
1	B	2105	TYR	2.8
1	A	2463	LEU	2.8
1	A	2118	ILE	2.7
1	B	2097	LEU	2.7
1	B	2474	PHE	2.4
1	A	2451	GLY	2.4
1	B	2285	ALA	2.4
1	A	2105	TYR	2.4
1	A	2078	VAL	2.4
1	B	2339	THR	2.3
1	B	2173	VAL	2.3
1	A	2077	PRO	2.3
1	B	2291	TRP	2.2
1	B	2134	LEU	2.2
1	A	2179	TYR	2.2
1	B	2084	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2398	LYS	2.1
1	B	2104	LEU	2.1
1	A	2158	ALA	2.0
1	A	2337	ASP	2.0
1	A	2462	VAL	2.0
1	B	2099	VAL	2.0
1	B	2135	PHE	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, 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	B-factors(Å^2)	Q<0.9
2	SO4	B	2501	5/5	0.87	0.11	48,59,59,62	0
2	SO4	A	2501	5/5	0.95	0.07	38,45,49,55	0

6.5 Other polymers (i)

There are no such residues in this entry.