Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 10:31 PM EST

PDB ID	:	3PZD
Title	:	Structure of the myosin X MyTH4-FERM/DCC complex
Authors	:	Wei, Z.; Yan, J.; Pan, L.; Zhang, M.
Deposited on	:	2010-12-14
Resolution	:	2.50 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:

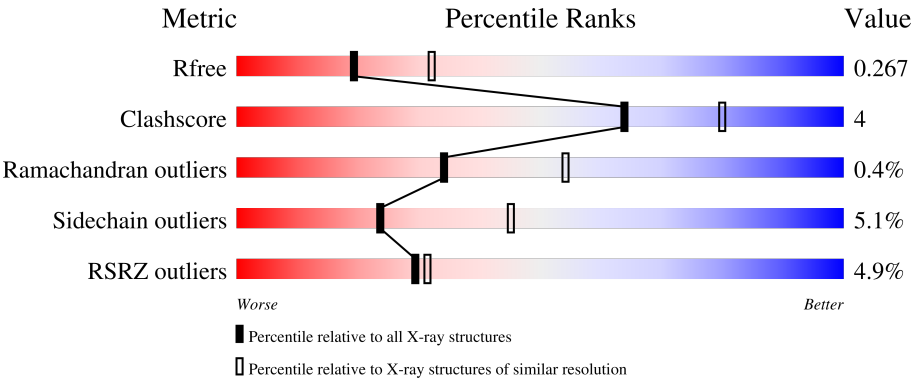
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	511	4% 84% 12%
2	B	36	11% 92% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4327 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 Myosin-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3964	2548	662	734	20	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1501	GLU	-	expression tag	UNP Q9HD67
A	1502	PHE	-	expression tag	UNP Q9HD67
A	?	-	PHE	deletion	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67
A	?	-	PRO	deletion	UNP Q9HD67
A	?	-	CYS	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	LEU	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	LYS	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67
A	?	-	SER	deletion	UNP Q9HD67
A	?	-	PHE	deletion	UNP Q9HD67
A	?	-	LEU	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	GLY	deletion	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67
A	?	-	LEU	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	SER	deletion	UNP Q9HD67
A	?	-	PHE	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67

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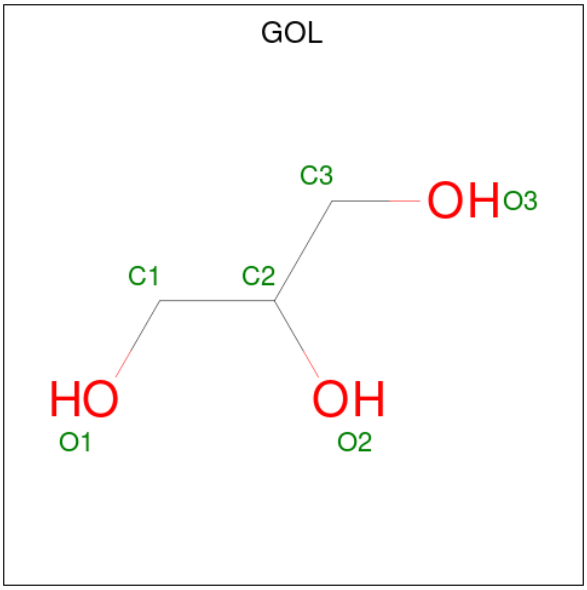
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q9HD67
A	?	-	SER	deletion	UNP Q9HD67
A	?	-	VAL	deletion	UNP Q9HD67
A	?	-	VAL	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	GLN	deletion	UNP Q9HD67
A	?	-	LYS	deletion	UNP Q9HD67
A	?	-	VAL	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67

- Molecule 2 is a protein called Netrin receptor DCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	0	0	0
			256	156	41	57	2			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			6	3	3			

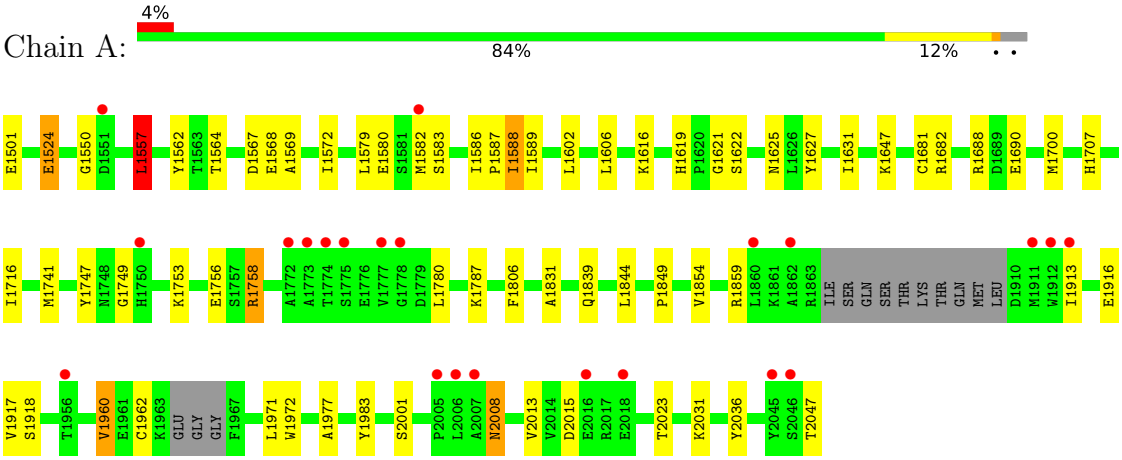
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	99	Total O 99 99	0	0
4	B	2	Total O 2 2	0	0

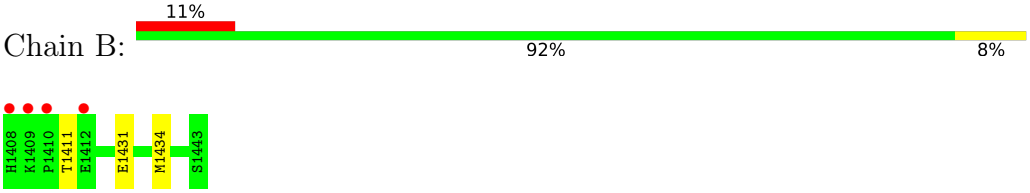
3 Residue-property plots (i)

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: Myosin-X



• Molecule 2: Netrin receptor DCC



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.17Å 49.53Å 92.81Å 90.00° 112.58° 90.00°	Depositor
Resolution (Å)	29.58 – 2.50 29.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.58-2.50) 99.4 (29.57-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.203 , 0.259 0.214 , 0.267	Depositor DCC
R_{free} test set	1242 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4327	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% 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: GOL

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	0.44	0/4056	0.56	1/5495 (0.0%)
2	B	0.36	0/258	0.50	0/349
All	All	0.43	0/4314	0.56	1/5844 (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	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	A	1557	LEU	CA-CB-CG	7.52	132.59	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1747	TYR	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	3964	0	3907	35	0
2	B	256	0	231	0	0
3	A	6	0	8	1	0
4	A	99	0	0	0	0
4	B	2	0	0	0	0
All	All	4327	0	4146	35	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 (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:1621:GLY:H	1:A:1625:ASN:HD22	1.18	0.91
1:A:1557:LEU:HD13	1:A:1562:TYR:HB2	1.66	0.77
1:A:1756:GLU:HB3	1:A:1758:ARG:NH2	2.04	0.72
1:A:1579:LEU:CD2	1:A:1631:ILE:HD11	2.22	0.70
1:A:1579:LEU:HD23	1:A:1631:ILE:HD11	1.74	0.68
1:A:1524:GLU:OE2	1:A:1616:LYS:NZ	2.29	0.64
1:A:1572:ILE:HG21	1:A:1606:LEU:HD11	1.83	0.61
1:A:1579:LEU:HD13	1:A:1588:ILE:HG12	1.83	0.60
1:A:2001:SER:HB3	1:A:2013:VAL:HB	1.83	0.60
1:A:1589:ILE:HG12	1:A:1631:ILE:HG12	1.86	0.57
1:A:1960:VAL:HG12	1:A:1971:LEU:HB2	1.86	0.57
1:A:1756:GLU:HB3	1:A:1758:ARG:HH21	1.69	0.56
1:A:1758:ARG:HH11	1:A:1758:ARG:HB3	1.76	0.51
1:A:1579:LEU:HA	1:A:1582:MET:HG3	1.94	0.50
1:A:1707:HIS:NE2	1:A:1787:LYS:HD3	2.27	0.50
1:A:1977:ALA:HA	1:A:2036:TYR:CD1	2.48	0.49
1:A:1619:HIS:CG	1:A:1622:SER:HB3	2.48	0.48
1:A:1700:MET:HG3	1:A:1716:ILE:HG13	1.94	0.48
1:A:1564:THR:OG1	1:A:1567:ASP:HB2	2.15	0.47
1:A:1749:GLY:HA3	1:A:1780:LEU:HD13	1.97	0.47
1:A:1572:ILE:HG21	1:A:1606:LEU:CD1	2.44	0.47
1:A:1831:ALA:HB1	1:A:1854:VAL:CG1	2.45	0.46
1:A:1682:ARG:HH22	1:A:1690:GLU:CD	2.18	0.45
1:A:2008:ASN:HB2	1:A:2023:THR:O	2.16	0.45
1:A:1564:THR:O	1:A:1568:GLU:HG2	2.17	0.45
1:A:1569:ALA:HB2	1:A:1602:LEU:CD2	2.46	0.45
1:A:1972:TRP:HB2	1:A:1983:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1839:GLN:OE1	1:A:1849:PRO:HD3	2.18	0.44
1:A:1606:LEU:HD12	1:A:1606:LEU:HA	1.88	0.43
1:A:1627:TYR:O	1:A:1631:ILE:HG13	2.17	0.43
1:A:1913:ILE:O	1:A:1917:VAL:HG23	2.19	0.43
1:A:1586:ILE:N	1:A:1587:PRO:HD2	2.34	0.43
1:A:1682:ARG:NH2	1:A:1690:GLU:OE2	2.50	0.42
1:A:1586:ILE:CG2	1:A:1688:ARG:HG3	2.51	0.41
1:A:1806:PHE:HA	3:A:1:GOL:H12	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	492/511 (96%)	471 (96%)	19 (4%)	2 (0%)	34 54
2	B	34/36 (94%)	31 (91%)	3 (9%)	0	100 100
All	All	526/547 (96%)	502 (95%)	22 (4%)	2 (0%)	34 54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1550	GLY
1	A	2008	ASN

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	428/454 (94%)	408 (95%)	20 (5%)	26 49
2	B	26/31 (84%)	23 (88%)	3 (12%)	5 11
All	All	454/485 (94%)	431 (95%)	23 (5%)	24 45

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1501	GLU
1	A	1524	GLU
1	A	1557	LEU
1	A	1580	GLU
1	A	1583	SER
1	A	1588	ILE
1	A	1647	LYS
1	A	1681	CYS
1	A	1741	MET
1	A	1753	LYS
1	A	1758	ARG
1	A	1844	LEU
1	A	1859	ARG
1	A	1916	GLU
1	A	1918	SER
1	A	1960	VAL
1	A	1962	CYS
1	A	2015	ASP
1	A	2031	LYS
1	A	2047	THR
2	B	1411	THR
2	B	1431	GLU
2	B	1434	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1525	GLN
1	A	1555	ASN
1	A	1625	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	GOL	A	1	-	5,5,5	0.64	0	5,5,5	0.53	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	GOL	A	1	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	GOL	O1-C1-C2-O2
3	A	1	GOL	C1-C2-C3-O3
3	A	1	GOL	O1-C1-C2-C3
3	A	1	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	GOL	1	0

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	498/511 (97%)	0.13	22 (4%) 34 37	19, 45, 96, 124	0
2	B	36/36 (100%)	0.59	4 (11%) 5 5	45, 71, 107, 116	0
All	All	534/547 (97%)	0.16	26 (4%) 29 31	19, 47, 98, 124	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1777	VAL	6.2
1	A	1862	ALA	6.2
1	A	2016	GLU	5.4
1	A	2007	ALA	4.5
1	A	1778	GLY	3.8
2	B	1409	LYS	3.8
1	A	2046	SER	3.7
1	A	1774	THR	3.7
1	A	2005	PRO	3.7
1	A	2006	LEU	3.6
1	A	1860	LEU	3.0
1	A	2045	TYR	2.9
2	B	1412	GLU	2.8
1	A	1551	ASP	2.8
2	B	1410	PRO	2.8
1	A	1913	ILE	2.7
1	A	1912	TRP	2.6
1	A	2018	GLU	2.5
1	A	1956	THR	2.4
1	A	1582	MET	2.3
1	A	1773	ALA	2.3
1	A	1750	HIS	2.2
2	B	1408	HIS	2.2
1	A	1772	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1775	SER	2.0
1	A	1911	MET	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, 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
3	GOL	A	1	6/6	0.91	0.24	32,37,39,40	0

6.5 Other polymers (i)

There are no such residues in this entry.