



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:07 PM UTC

PDB ID : 8TEE / pdb_00008tee
Title : Crystal structure of Kindlin2 in complex with K794Q mutated beta1 integrin
Authors : Zhang, P.F.; Wu, J.H.
Deposited on : 2023-07-06
Resolution : 2.49 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

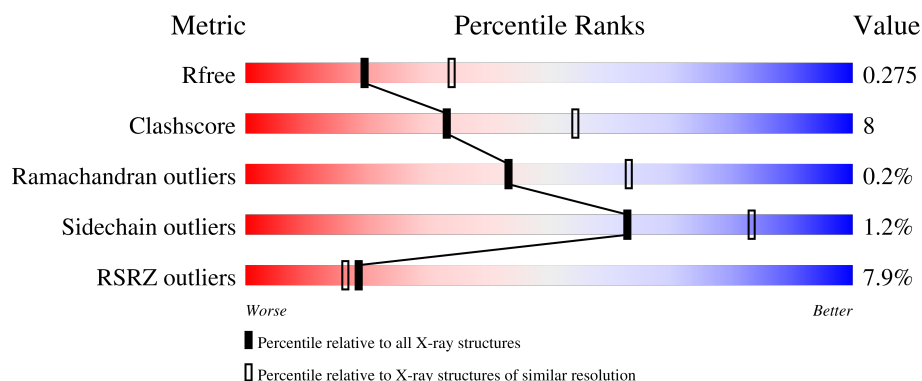
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	504	6% 68% 15% 17%
1	B	504	7% 68% 17% 15%
2	C	15	67% 13% 20%
2	D	15	13% 47% 27% 27%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6827 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 Fermitin family homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3233	2080	547	587	19			
1	B	429	Total	C	N	O	S	0	0	0
			3326	2137	561	606	22			

- Molecule 2 is a protein called Integrin beta-1.

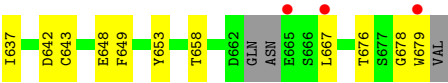
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			89	56	14	19			
2	D	11	Total	C	N	O	0	0	0
			81	52	13	16			

There are 2 discrepancies between the modelled and reference sequences:

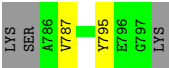
Chain	Residue	Modelled	Actual	Comment	Reference
C	794	GLN	LYS	engineered mutation	UNP P09055
D	794	GLN	LYS	engineered mutation	UNP P09055

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	39	Total	O	0	0
			39	39		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		



● Molecule 2: Integrin beta-1



● Molecule 2: Integrin beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 98.29Å 76.00Å 90.00° 96.42° 90.00°	Depositor
Resolution (Å)	29.94 – 2.49 29.94 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.94-2.49) 97.8 (29.94-2.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.227 , 0.275 0.227 , 0.275	Depositor DCC
R_{free} test set	1858 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6827	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/3305	0.33	0/4497
1	B	0.12	0/3404	0.30	0/4635
2	C	0.15	0/90	0.46	0/124
2	D	0.16	0/82	0.39	0/114
All	All	0.13	0/6881	0.32	0/9370

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	3233	0	3049	46	1
1	B	3326	0	3132	57	1
2	C	89	0	84	2	0
2	D	81	0	77	5	0
3	A	57	0	0	0	0
3	B	39	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	6827	0	6342	102	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 8.

All (102) 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:274:PHE:H	1:A:297:GLN:HE22	1.12	0.97
1:B:36:THR:HG23	1:B:38:GLU:H	1.45	0.81
1:B:514:THR:HG21	1:B:540:LEU:HD21	1.63	0.80
1:B:221:LEU:HB3	1:B:289:ILE:HD11	1.65	0.76
1:B:36:THR:HG22	1:B:39:VAL:HG23	1.65	0.75
1:A:274:PHE:N	1:A:297:GLN:HE22	1.88	0.67
1:B:612:MET:O	2:D:792:ASN:ND2	2.29	0.65
1:A:41:ILE:O	1:A:45:MET:HG3	1.97	0.64
1:B:678:GLY:HA2	2:D:788:THR:HG21	1.80	0.64
1:B:518:PRO:HD2	1:B:521:LEU:HD11	1.79	0.63
1:B:623:MET:SD	1:B:635:SER:OG	2.57	0.62
1:B:46:LEU:O	1:B:50:GLU:HG3	2.01	0.61
1:A:36:THR:HG22	1:A:39:VAL:HG12	1.82	0.61
1:B:119:VAL:HG22	1:B:255:SER:HA	1.83	0.60
1:B:221:LEU:HB3	1:B:289:ILE:CD1	2.31	0.60
1:B:113:VAL:HG21	1:B:126:ILE:HD11	1.84	0.60
1:B:95:GLN:HB3	1:B:114:ASN:OD1	2.03	0.58
1:B:619:TRP:NE1	2:D:788:THR:OG1	2.28	0.57
1:A:274:PHE:H	1:A:297:GLN:NE2	1.93	0.57
1:B:559:ILE:O	1:B:563:GLN:HG3	2.05	0.57
1:A:530:TYR:HB2	1:A:535:ILE:HD11	1.89	0.55
1:A:336:LEU:HD23	1:A:336:LEU:H	1.72	0.55
1:B:26:ASP:OD2	1:B:61:HIS:NE2	2.38	0.55
1:B:648:GLU:HG3	1:B:676:THR:HB	1.89	0.54
1:B:82:CYS:HB2	1:B:84:ILE:HG13	1.90	0.54
1:B:48:LEU:O	1:B:52:LEU:HG	2.08	0.53
1:A:519:GLU:HA	1:A:527:LEU:HD11	1.90	0.53
1:B:107:LYS:HB3	1:B:220:ILE:HD13	1.91	0.52
1:B:100:ARG:HE	1:B:108:TYR:HB3	1.74	0.52
1:B:68:LYS:HB3	1:B:70:THR:HG22	1.92	0.51
1:B:40:HIS:HA	1:B:78:THR:HA	1.92	0.51
1:B:336:LEU:O	1:B:514:THR:N	2.39	0.51
1:A:130:PHE:O	1:A:289:ILE:HD13	2.09	0.51
1:B:257:ARG:HH21	1:B:261:GLU:HB3	1.75	0.50
1:A:600:THR:HG23	1:A:602:ASP:H	1.75	0.50
1:A:616:ASN:OD1	1:A:625:THR:HB	2.13	0.49
1:B:227:VAL:HG11	1:B:233:LEU:HB2	1.93	0.49
1:B:519:GLU:OE2	1:B:536:THR:OG1	2.25	0.49
1:B:119:VAL:HG13	1:B:257:ARG:O	2.13	0.49
1:B:334:ASN:ND2	1:B:544:GLN:HG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HD13	1:B:16:GLY:HA3	1.95	0.48
1:A:325:ASN:O	1:A:329:ILE:HG13	2.15	0.47
1:B:104:PRO:HB3	1:B:297:GLN:HB2	1.97	0.47
1:A:56:LYS:HB3	1:A:58:TRP:NE1	2.30	0.47
1:B:250:GLN:HG2	1:B:642:ASP:OD1	2.15	0.46
1:B:136:GLU:HB3	1:B:667:LEU:HD21	1.97	0.46
1:A:303:LEU:HD12	1:A:304:LEU:HG	1.98	0.46
1:A:663:GLN:O	1:A:665:GLU:N	2.46	0.46
1:B:45:MET:HE3	1:B:92:PHE:HE1	1.81	0.46
1:A:327:LEU:HA	1:A:330:MET:HG3	1.98	0.46
1:A:53:ASP:HB3	1:A:56:LYS:HB2	1.98	0.45
1:A:590:TYR:HA	1:A:653:TYR:CD1	2.52	0.45
1:B:605:LYS:HD2	1:B:607:TRP:CE2	2.51	0.45
1:A:275:LYS:HE2	1:A:276:TYR:CZ	2.52	0.45
1:B:275:LYS:HE3	1:B:649:PHE:CE2	2.50	0.45
1:B:623:MET:HG3	1:B:637:ILE:HG13	1.98	0.45
1:A:36:THR:HG23	1:A:38:GLU:H	1.82	0.45
1:A:94:PRO:O	1:A:97:LYS:NZ	2.47	0.45
1:A:613:LYS:HB2	1:A:613:LYS:HE3	1.64	0.45
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.81	0.45
1:B:227:VAL:HG21	1:B:233:LEU:HD13	1.99	0.44
1:A:99:LEU:HD21	1:A:270:LEU:HD12	2.00	0.44
1:B:122:ALA:O	1:B:126:ILE:HD12	2.18	0.44
1:A:27:LEU:HD11	1:A:58:TRP:HH2	1.82	0.44
1:B:130:PHE:CD1	1:B:221:LEU:HD11	2.53	0.44
1:A:54:VAL:HG22	1:B:545:ASN:OD1	2.18	0.43
1:A:233:LEU:O	1:A:237:PHE:N	2.51	0.43
1:B:119:VAL:HA	1:B:122:ALA:HB3	2.00	0.43
1:B:574:ILE:H	1:B:574:ILE:HG12	1.61	0.43
1:A:314:MET:HE2	1:A:314:MET:HB2	1.89	0.43
1:A:77:TRP:HE3	1:A:82:CYS:SG	2.42	0.43
1:A:79:LEU:O	1:A:83:GLY:N	2.52	0.43
1:A:296:GLU:O	1:A:300:TRP:HD1	2.01	0.43
1:B:232:ILE:O	1:B:236:MET:HG3	2.19	0.43
1:A:224:SER:HB2	1:A:292:ASN:OD1	2.18	0.42
1:A:277:TYR:CG	1:A:569:GLY:HA2	2.54	0.42
1:B:277:TYR:CG	1:B:569:GLY:HA2	2.54	0.42
1:B:243:LEU:HD13	1:B:598:ALA:HB1	2.01	0.42
1:A:299:LYS:O	1:A:303:LEU:HG	2.18	0.42
1:A:302:LEU:HD21	1:A:565:LEU:HD11	2.02	0.42
1:B:336:LEU:C	1:B:514:THR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TRP:CE3	1:A:303:LEU:HD11	2.55	0.41
1:B:276:TYR:HB3	1:B:653:TYR:CE1	2.55	0.41
1:B:658:THR:HG22	2:D:794:GLN:NE2	2.35	0.41
1:A:258:SER:O	1:A:262:GLN:HG3	2.20	0.41
1:A:673:TYR:O	1:A:677:SER:OG	2.34	0.41
1:A:334:ASN:O	1:A:514:THR:HB	2.20	0.41
1:A:617:VAL:O	2:C:787:VAL:HA	2.20	0.41
1:B:679:TRP:N	1:B:679:TRP:CD1	2.88	0.41
1:A:316:MET:HE3	1:A:316:MET:HB3	1.83	0.41
1:A:629:ALA:HB2	2:C:795:TYR:OH	2.21	0.41
1:B:275:LYS:HE2	1:B:276:TYR:CZ	2.55	0.41
1:A:120:PHE:HB2	1:A:255:SER:HB3	2.01	0.41
1:B:41:ILE:O	1:B:45:MET:HG3	2.19	0.41
1:B:607:TRP:HB3	1:B:628:PHE:CE2	2.56	0.41
1:A:545:ASN:OD1	1:B:54:VAL:HG22	2.21	0.41
1:A:605:LYS:HE2	1:A:607:TRP:NE1	2.36	0.41
1:B:136:GLU:OE2	1:B:136:GLU:N	2.35	0.40
1:A:607:TRP:HB3	1:A:628:PHE:CE1	2.57	0.40
1:B:102:GLN:HB3	1:B:271:LEU:HD23	2.02	0.40
1:B:335:HIS:O	1:B:513:THR:N	2.52	0.40
2:D:795:TYR:CD1	2:D:795:TYR:C	2.98	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)
1:A:530:TYR:OH	1:B:311:GLU:OE1[1_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	412/504 (82%)	386 (94%)	24 (6%)	2 (0%)	24	43
1	B	423/504 (84%)	403 (95%)	20 (5%)	0	100	100
2	C	10/15 (67%)	8 (80%)	2 (20%)	0	100	100
2	D	9/15 (60%)	9 (100%)	0	0	100	100
All	All	854/1038 (82%)	806 (94%)	46 (5%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	664	ASN

5.3.2 Protein sidechains ⓘ

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	323/449 (72%)	319 (99%)	4 (1%)	63	83
1	B	336/449 (75%)	332 (99%)	4 (1%)	63	83
2	C	10/13 (77%)	10 (100%)	0	100	100
2	D	9/13 (69%)	9 (100%)	0	100	100
All	All	678/924 (73%)	670 (99%)	8 (1%)	63	83

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

Mol	Chain	Res	Type
1	A	39	VAL
1	A	113	VAL
1	A	202	SER
1	A	667	LEU
1	B	6	ILE
1	B	126	ILE
1	B	220	ILE
1	B	643	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	95	GLN
1	A	297	GLN
1	A	572	HIS
1	B	293	GLN
1	B	323	HIS
1	B	517	ASN
1	B	560	GLN
1	B	572	HIS
1	B	614	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](#)

There are no ligands in this entry.

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	420/504 (83%)	0.59	32 (7%) 20 17	41, 63, 126, 162	0
1	B	429/504 (85%)	0.60	35 (8%) 17 15	42, 68, 114, 153	0
2	C	12/15 (80%)	0.59	0 100 100	56, 61, 78, 79	0
2	D	11/15 (73%)	1.42	2 (18%) 3 2	79, 94, 113, 113	0
All	All	872/1038 (84%)	0.61	69 (7%) 18 16	41, 66, 121, 162	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ALA	5.6
1	A	227	VAL	5.4
1	B	519	GLU	5.2
1	B	517	ASN	4.8
1	A	17	THR	4.2
1	A	286	TYR	3.7
1	B	218	PRO	3.6
1	A	680	VAL	3.5
1	A	79	LEU	3.5
1	B	520	CYS	3.3
1	B	266	GLU	3.3
1	B	239	PRO	3.2
1	A	228	THR	3.1
1	B	59	SER	3.1
1	B	237	PHE	3.1
1	A	679	TRP	3.1
1	B	334	ASN	3.0
1	A	20	LEU	3.0
1	A	336	LEU	3.0
1	B	336	LEU	2.9
1	A	58	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	230	PRO	2.8
1	B	679	TRP	2.7
1	A	662	ASP	2.7
2	D	787	VAL	2.7
1	A	18	TRP	2.7
1	B	515	ASP	2.6
1	B	6	ILE	2.5
1	A	335	HIS	2.5
1	A	199	SER	2.5
1	B	518	PRO	2.4
1	B	532	SER	2.4
1	A	264	VAL	2.4
1	B	265	LYS	2.4
1	B	580	GLY	2.4
1	B	80	ASP	2.4
1	B	76	HIS	2.4
1	A	522	VAL	2.4
1	B	516	VAL	2.4
1	B	5	GLY	2.3
1	A	15	ASP	2.3
1	B	4	ASP	2.3
1	B	527	LEU	2.3
1	A	222	ALA	2.3
1	A	220	ILE	2.3
1	B	513	THR	2.3
1	B	41	ILE	2.3
1	B	286	TYR	2.3
1	A	660	ALA	2.3
1	B	225	GLN	2.3
1	B	233	LEU	2.3
1	B	54	VAL	2.3
1	A	32	THR	2.2
1	A	237	PHE	2.2
1	A	16	GLY	2.2
1	B	667	LEU	2.2
1	A	200	PRO	2.2
1	A	37	GLY	2.2
1	B	521	LEU	2.2
1	B	665	GLU	2.2
1	B	147	PRO	2.2
1	A	266	GLU	2.1
1	B	578	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	676	THR	2.1
1	A	229	SER	2.1
1	A	516	VAL	2.1
2	D	795	TYR	2.0
1	B	49	VAL	2.0
1	A	242	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.