



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:17 PM GMT

PDB ID : 1A38  
Title : 14-3-3 PROTEIN ZETA BOUND TO R18 PEPTIDE  
Authors : Petosa, C.; Masters, S.C.; Pohl, J.; Wang, B.; Fu, H.; Liddington, R.C.  
Deposited on : 1998-01-28  
Resolution : 3.35 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

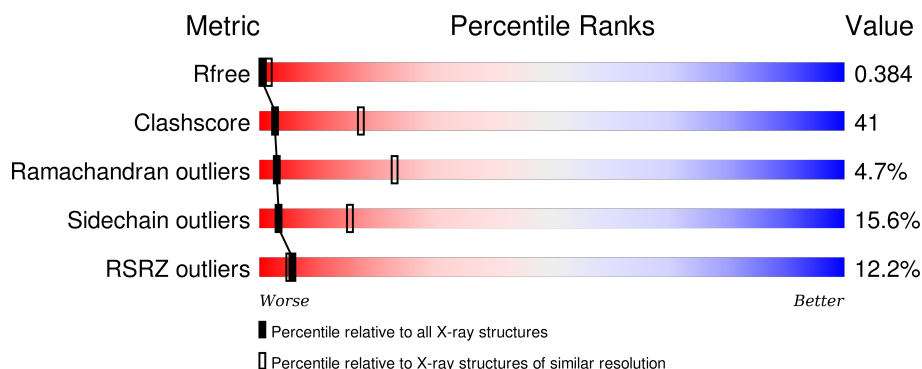
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	245	<div> <div>10%</div> <div>29%</div> <div>47%</div> <div>11%</div> <div>12%</div> </div>
1	B	245	<div> <div>10%</div> <div>30%</div> <div>46%</div> <div>11%</div> <div>12%</div> </div>
2	P	20	<div> <div>15%</div> <div>5%</div> <div>20%</div> <div>75%</div> </div>
2	Q	20	<div> <div>10%</div> <div>5%</div> <div>20%</div> <div>75%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3554 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 14-3-3 PROTEIN ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1730	1085	293	342	10			
1	B	216	Total	C	N	O	S	0	0	0
			1730	1085	293	342	10			

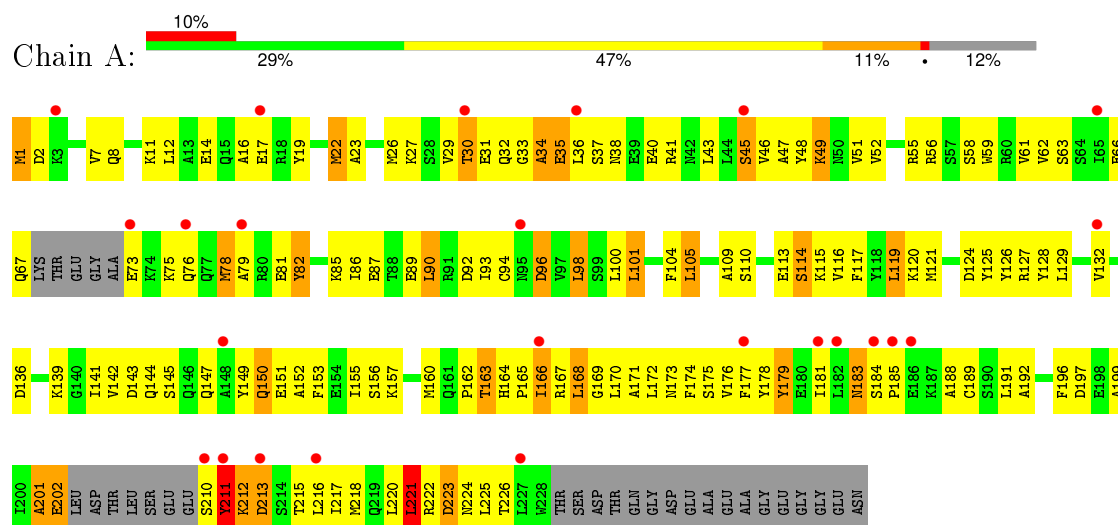
- Molecule 2 is a protein called R18 PEPTIDE (PHCVPRDLSWLDLEANMCLP).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			47	32	6	9			
2	Q	5	Total	C	N	O	0	0	0
			47	32	6	9			

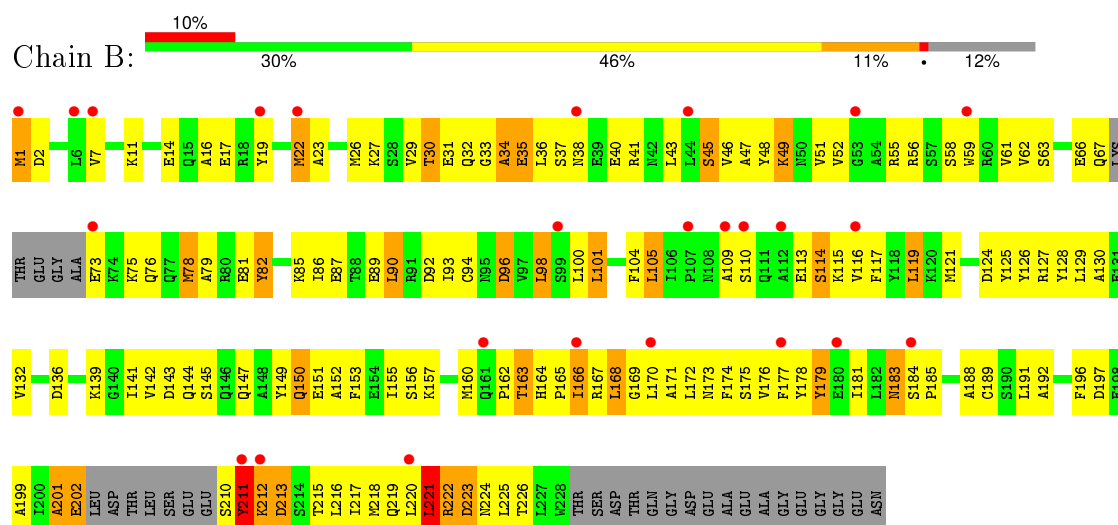
### 3 Residue-property plots

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: 14-3-3 PROTEIN ZETA

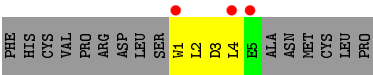


#### • Molecule 1: 14-3-3 PROTEIN ZETA

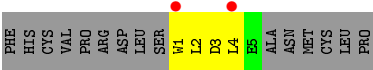


#### • Molecule 2: R18 PEPTIDE (PHCVPRDLSWLDLEANMCLP)





● Molecule 2: R18 PEPTIDE (PHCVPRDLSWLDLEANMCLP)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.52Å 95.52Å 235.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.35 29.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.35) 95.4 (29.04-3.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 3.11Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.330 , 0.390 0.367 , 0.384	Depositor DCC
$R_{free}$ test set	1710 reflections (11.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.2	EDS
Estimated twinning fraction	0.449 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 20975 reflections	Xtriage
$F_o, F_c$ correlation	0.68	EDS
Total number of atoms	3554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	0.55	0/1751	0.92	3/2348 (0.1%)
1	B	0.55	0/1751	0.92	3/2348 (0.1%)
2	P	0.71	0/48	0.88	0/65
2	Q	0.72	0/48	0.88	0/65
All	All	0.55	0/3598	0.92	6/4826 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	LEU	CA-CB-CG	7.83	133.32	115.30
1	A	221	LEU	CA-CB-CG	7.83	133.31	115.30
1	B	202	GLU	N-CA-C	5.43	125.67	111.00
1	A	202	GLU	N-CA-C	5.42	125.64	111.00
1	B	19	TYR	N-CA-C	5.31	125.34	111.00
1	A	19	TYR	N-CA-C	5.30	125.32	111.00

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	1730	0	1726	144	0
1	B	1730	0	1726	145	0
2	P	47	0	44	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	47	0	44	7	0
All	All	3554	0	3540	290	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 41.

All (290) 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:220:LEU:HD23	2:P:4:LEU:HD11	1.49	0.94
1:B:220:LEU:HD23	2:Q:4:LEU:HD11	1.49	0.92
1:A:89:GLU:O	1:A:93:ILE:HG12	1.77	0.85
1:B:89:GLU:O	1:B:93:ILE:HG12	1.77	0.84
1:B:178:TYR:HB2	1:B:188:ALA:HB2	1.59	0.84
1:A:178:TYR:HB2	1:A:188:ALA:HB2	1.59	0.83
1:B:30:THR:OG1	1:B:100:LEU:HD23	1.78	0.83
1:A:30:THR:OG1	1:A:100:LEU:HD23	1.78	0.82
1:A:52:VAL:O	1:A:56:ARG:HG3	1.80	0.82
1:B:52:VAL:O	1:B:56:ARG:HG3	1.80	0.81
1:A:55:ARG:HB3	1:A:90:LEU:HD22	1.64	0.80
1:A:26:MET:O	1:A:30:THR:HG23	1.83	0.79
1:B:101:LEU:HD12	1:B:105:LEU:HD23	1.63	0.79
1:A:101:LEU:HD12	1:A:105:LEU:HD23	1.63	0.79
1:B:55:ARG:HB3	1:B:90:LEU:HD22	1.64	0.79
1:A:48:TYR:O	1:A:52:VAL:HG12	1.83	0.79
1:B:26:MET:O	1:B:30:THR:HG23	1.83	0.78
1:B:48:TYR:O	1:B:52:VAL:HG12	1.83	0.78
1:B:177:PHE:O	1:B:181:ILE:HB	1.83	0.78
1:B:75:LYS:O	1:B:78:MET:HG3	1.84	0.78
1:A:75:LYS:O	1:A:78:MET:HG3	1.84	0.78
1:A:177:PHE:O	1:A:181:ILE:HB	1.83	0.76
1:B:52:VAL:HG11	1:B:125:TYR:CE1	2.23	0.73
1:A:217:ILE:O	1:A:221:LEU:HD23	1.89	0.73
1:B:7:VAL:O	1:B:11:LYS:HG2	1.88	0.72
1:A:7:VAL:O	1:A:11:LYS:HG2	1.88	0.72
1:B:151:GLU:O	1:B:155:ILE:HG13	1.89	0.72
1:A:151:GLU:O	1:A:155:ILE:HG13	1.89	0.72
1:A:52:VAL:HG11	1:A:125:TYR:CE1	2.23	0.72
1:B:217:ILE:O	1:B:221:LEU:HD23	1.89	0.72
1:B:100:LEU:HD12	1:B:100:LEU:H	1.57	0.70
1:A:52:VAL:HG11	1:A:125:TYR:HE1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:H	1:A:100:LEU:HD12	1.57	0.69
1:B:220:LEU:CD2	2:Q:4:LEU:HD11	2.22	0.69
1:B:116:VAL:HG23	1:B:152:ALA:HB1	1.75	0.69
1:A:220:LEU:CD2	2:P:4:LEU:HD11	2.22	0.68
1:A:116:VAL:HG23	1:A:152:ALA:HB1	1.75	0.68
1:B:52:VAL:HG11	1:B:125:TYR:HE1	1.58	0.68
1:B:115:LYS:O	1:B:119:LEU:HD12	1.95	0.67
1:A:115:LYS:O	1:A:119:LEU:HD12	1.95	0.67
1:A:58:SER:O	1:A:62:VAL:HG12	1.95	0.66
1:B:58:SER:O	1:B:62:VAL:HG12	1.95	0.66
1:B:165:PRO:HG3	1:B:213:ASP:HB2	1.77	0.66
1:B:173:ASN:O	1:B:176:VAL:HG12	1.96	0.66
1:A:173:ASN:O	1:A:176:VAL:HG12	1.96	0.66
1:A:101:LEU:CD1	1:A:105:LEU:HD23	2.25	0.65
1:B:101:LEU:CD1	1:B:105:LEU:HD23	2.25	0.65
1:A:165:PRO:HG3	1:A:213:ASP:HB2	1.77	0.65
1:B:43:LEU:O	1:B:46:VAL:HG12	1.98	0.64
1:B:22:MET:SD	1:B:47:ALA:HB2	2.38	0.64
1:B:45:SER:HG	1:B:117:PHE:HZ	1.46	0.63
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.81	0.63
1:A:35:GLU:OE1	1:A:35:GLU:HA	1.99	0.63
2:P:1:TRP:HD1	2:P:2:LEU:H	1.46	0.63
1:A:22:MET:SD	1:A:47:ALA:HB2	2.38	0.63
1:B:101:LEU:HA	1:B:105:LEU:HB2	1.81	0.63
1:A:185:PRO:O	1:A:189:CYS:SG	2.55	0.62
1:B:101:LEU:HD21	1:B:121:MET:HG2	1.80	0.62
1:A:143:ASP:O	1:A:147:GLN:HG3	2.00	0.62
1:A:43:LEU:O	1:A:46:VAL:HG12	1.98	0.62
1:A:192:ALA:HB1	1:A:225:LEU:HD11	1.82	0.62
1:B:143:ASP:O	1:B:147:GLN:HG3	2.00	0.62
1:B:59:TRP:HE1	1:B:87:GLU:HG3	1.65	0.62
1:B:192:ALA:HB1	1:B:225:LEU:HD11	1.82	0.61
1:A:101:LEU:HD21	1:A:121:MET:HG2	1.80	0.61
1:A:59:TRP:HE1	1:A:87:GLU:HG3	1.65	0.61
1:A:94:CYS:O	1:A:98:LEU:HB2	2.00	0.61
1:B:94:CYS:O	1:B:98:LEU:HB2	2.00	0.61
2:Q:1:TRP:HD1	2:Q:2:LEU:H	1.47	0.61
1:B:35:GLU:HA	1:B:35:GLU:OE1	1.99	0.61
1:B:66:GLU:HB2	1:B:79:ALA:HB1	1.81	0.61
1:B:185:PRO:O	1:B:189:CYS:SG	2.55	0.61
1:A:201:ALA:O	1:A:202:GLU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:HA	1:A:152:ALA:HB1	1.83	0.61
1:A:66:GLU:HB2	1:A:79:ALA:HB1	1.81	0.61
1:B:116:VAL:HA	1:B:152:ALA:HB1	1.83	0.61
1:A:51:VAL:HG13	1:A:55:ARG:NH1	2.17	0.59
1:A:216:LEU:O	1:A:220:LEU:HD13	2.03	0.59
1:A:124:ASP:O	1:A:127:ARG:HB3	2.03	0.59
1:B:201:ALA:O	1:B:202:GLU:HB2	2.01	0.59
1:B:51:VAL:HG13	1:B:55:ARG:NH1	2.17	0.59
1:B:192:ALA:CB	1:B:225:LEU:HD11	2.33	0.59
1:B:124:ASP:O	1:B:127:ARG:HB3	2.03	0.59
1:B:216:LEU:O	1:B:220:LEU:HD13	2.02	0.59
1:A:45:SER:HG	1:A:117:PHE:HZ	1.49	0.58
1:A:169:GLY:HA3	2:P:2:LEU:HD11	1.84	0.58
1:A:192:ALA:CB	1:A:225:LEU:HD11	2.33	0.58
1:B:162:PRO:C	1:B:164:HIS:H	2.07	0.58
1:B:169:GLY:HA3	2:Q:2:LEU:HD11	1.84	0.58
1:B:101:LEU:HD21	1:B:121:MET:HB3	1.86	0.58
1:B:213:ASP:O	1:B:217:ILE:HG13	2.04	0.58
1:A:8:GLN:HE21	1:B:78:MET:HE2	1.69	0.58
1:A:30:THR:C	1:A:32:GLN:H	2.07	0.57
1:B:73:GLU:O	1:B:76:GLN:HB3	2.04	0.57
1:A:101:LEU:HD21	1:A:121:MET:HB3	1.86	0.57
1:A:139:LYS:HA	1:A:142:VAL:HG12	1.86	0.57
1:B:87:GLU:HG2	1:B:132:VAL:HG13	1.87	0.57
1:A:38:ASN:HA	1:A:41:ARG:HB3	1.87	0.57
1:A:163:THR:O	1:A:163:THR:HG22	2.05	0.57
1:A:162:PRO:C	1:A:164:HIS:H	2.07	0.56
1:A:73:GLU:O	1:A:76:GLN:HB3	2.04	0.56
1:A:213:ASP:O	1:A:217:ILE:HG13	2.04	0.56
1:B:38:ASN:HA	1:B:41:ARG:HB3	1.87	0.56
1:A:129:LEU:HB3	1:A:141:ILE:HG21	1.87	0.56
1:B:212:LYS:O	1:B:215:THR:HB	2.06	0.56
1:A:87:GLU:HG2	1:A:132:VAL:HG13	1.87	0.56
1:B:30:THR:C	1:B:32:GLN:H	2.07	0.56
1:A:150:GLN:O	1:A:150:GLN:HG3	2.05	0.56
1:B:163:THR:HG22	1:B:163:THR:O	2.05	0.56
1:B:139:LYS:HA	1:B:142:VAL:HG12	1.86	0.56
1:A:212:LYS:O	1:A:215:THR:HB	2.06	0.56
1:B:129:LEU:HB3	1:B:141:ILE:HG21	1.87	0.55
1:B:150:GLN:O	1:B:150:GLN:HG3	2.05	0.55
1:B:59:TRP:NE1	1:B:87:GLU:HG3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD12	1:B:174:PHE:HB2	1.88	0.54
1:A:170:LEU:HD12	1:A:174:PHE:HB2	1.88	0.54
1:A:59:TRP:NE1	1:A:87:GLU:HG3	2.22	0.53
1:A:124:ASP:HA	1:A:149:TYR:OH	2.08	0.53
1:A:162:PRO:O	1:A:168:LEU:HD13	2.08	0.53
1:B:168:LEU:HB3	1:B:217:ILE:HG21	1.90	0.53
1:B:124:ASP:HA	1:B:149:TYR:OH	2.08	0.53
1:A:168:LEU:HB3	1:A:217:ILE:HG21	1.90	0.53
1:B:169:GLY:O	1:B:172:LEU:HB3	2.08	0.53
1:B:162:PRO:O	1:B:168:LEU:HD13	2.08	0.53
1:B:116:VAL:HG21	1:B:156:SER:HB3	1.91	0.52
1:B:87:GLU:CD	1:B:132:VAL:HG13	2.30	0.52
1:A:126:TYR:CD1	1:A:144:GLN:HB3	2.45	0.52
1:B:126:TYR:CE1	1:B:144:GLN:HB3	2.45	0.52
1:B:87:GLU:HG2	1:B:132:VAL:CG1	2.40	0.52
1:A:87:GLU:CD	1:A:132:VAL:HG13	2.30	0.52
1:A:87:GLU:HG2	1:A:132:VAL:CG1	2.40	0.52
1:A:116:VAL:HG21	1:A:156:SER:HB3	1.91	0.52
1:A:61:VAL:HG13	1:A:62:VAL:H	1.75	0.52
1:B:61:VAL:HG13	1:B:62:VAL:H	1.75	0.52
1:A:169:GLY:O	1:A:172:LEU:HB3	2.09	0.52
1:A:126:TYR:CE1	1:A:144:GLN:HB3	2.45	0.52
1:B:87:GLU:CG	1:B:132:VAL:HG13	2.40	0.52
1:A:125:TYR:HA	1:A:128:TYR:CD2	2.45	0.52
1:A:87:GLU:CG	1:A:132:VAL:HG13	2.40	0.52
1:B:126:TYR:CD1	1:B:144:GLN:HB3	2.45	0.52
1:B:109:ALA:HB1	1:B:114:SER:HB2	1.93	0.51
1:A:98:LEU:HD11	1:A:126:TYR:CD2	2.46	0.51
1:B:98:LEU:HD11	1:B:126:TYR:CD2	2.46	0.51
1:A:14:GLU:HB2	1:A:22:MET:SD	2.51	0.51
1:B:14:GLU:HB2	1:B:22:MET:SD	2.51	0.50
1:A:109:ALA:HB1	1:A:114:SER:HB2	1.93	0.50
1:B:125:TYR:HA	1:B:128:TYR:CD2	2.45	0.50
1:A:8:GLN:CD	1:B:75:LYS:HD2	2.31	0.50
1:B:14:GLU:C	1:B:16:ALA:H	2.15	0.50
1:B:153:PHE:O	1:B:157:LYS:HB2	2.12	0.50
1:A:14:GLU:C	1:A:16:ALA:H	2.15	0.49
1:A:192:ALA:O	1:A:196:PHE:HB3	2.13	0.49
1:A:178:TYR:HD1	1:A:184:SER:HB3	1.77	0.49
1:A:76:GLN:O	1:A:79:ALA:HB3	2.13	0.49
1:A:152:ALA:HA	1:A:155:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLN:O	1:B:79:ALA:HB3	2.13	0.49
1:B:162:PRO:O	1:B:168:LEU:HD22	2.13	0.48
1:B:173:ASN:HA	1:B:176:VAL:HG12	1.95	0.48
1:A:8:GLN:HE21	1:B:78:MET:CE	2.26	0.48
1:A:45:SER:O	1:A:49:LYS:HB3	2.14	0.48
1:A:220:LEU:H	1:A:220:LEU:CD1	2.27	0.48
1:B:178:TYR:HD1	1:B:184:SER:HB3	1.77	0.48
1:B:63:SER:O	1:B:67:GLN:N	2.45	0.48
1:B:45:SER:O	1:B:49:LYS:HB3	2.14	0.48
1:B:152:ALA:HA	1:B:155:ILE:HB	1.94	0.48
1:B:213:ASP:HA	1:B:216:LEU:HD12	1.96	0.48
1:A:153:PHE:O	1:A:157:LYS:HB2	2.12	0.48
1:B:23:ALA:HB1	1:B:48:TYR:CE2	2.49	0.48
1:B:223:ASP:O	1:B:226:THR:HB	2.14	0.48
1:B:221:LEU:O	1:B:224:ASN:HB2	2.14	0.48
1:B:172:LEU:O	1:B:175:SER:HB3	2.14	0.48
1:B:192:ALA:O	1:B:196:PHE:HB3	2.13	0.47
1:A:211:TYR:CD1	1:A:212:LYS:N	2.82	0.47
1:A:63:SER:O	1:A:67:GLN:N	2.45	0.47
1:A:23:ALA:HB1	1:A:48:TYR:CE2	2.49	0.47
1:A:213:ASP:HA	1:A:216:LEU:HD12	1.96	0.47
1:A:117:PHE:HB2	1:A:166:ILE:HD11	1.96	0.47
1:A:162:PRO:O	1:A:168:LEU:HD22	2.13	0.47
1:B:61:VAL:HG13	1:B:62:VAL:N	2.29	0.47
1:A:221:LEU:O	1:A:224:ASN:HB2	2.14	0.47
1:B:220:LEU:CD1	1:B:220:LEU:H	2.27	0.47
1:A:173:ASN:HA	1:A:176:VAL:HG12	1.95	0.47
1:B:117:PHE:HB2	1:B:166:ILE:HD11	1.96	0.47
1:A:172:LEU:O	1:A:175:SER:HB3	2.14	0.47
1:B:211:TYR:CD1	1:B:212:LYS:N	2.82	0.47
2:P:1:TRP:CD1	2:P:2:LEU:N	2.80	0.47
1:A:217:ILE:O	1:A:221:LEU:CD2	2.61	0.47
2:Q:1:TRP:CD1	2:Q:2:LEU:N	2.80	0.46
1:A:220:LEU:N	1:A:220:LEU:CD1	2.78	0.46
1:B:220:LEU:N	1:B:220:LEU:CD1	2.78	0.46
1:A:223:ASP:O	1:A:226:THR:HB	2.14	0.46
1:A:61:VAL:HG13	1:A:62:VAL:N	2.29	0.46
1:A:169:GLY:HA3	2:P:2:LEU:CD1	2.46	0.46
1:B:217:ILE:O	1:B:221:LEU:CD2	2.61	0.46
1:A:82:TYR:O	1:A:86:ILE:HG13	2.16	0.45
1:B:31:GLU:HA	1:B:104:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:SER:HB3	1:B:177:PHE:CE1	2.51	0.45
2:Q:2:LEU:HG	2:Q:3:ASP:N	2.31	0.45
1:A:31:GLU:HA	1:A:104:PHE:CZ	2.51	0.45
1:A:27:LYS:HA	1:A:100:LEU:HD21	1.98	0.45
1:A:116:VAL:HA	1:A:152:ALA:CB	2.47	0.45
1:B:92:ASP:O	1:B:96:ASP:HB2	2.17	0.45
1:B:82:TYR:O	1:B:86:ILE:HG13	2.16	0.45
1:B:37:SER:HB3	1:B:40:GLU:HG3	1.98	0.45
1:B:101:LEU:HD21	1:B:121:MET:CG	2.44	0.45
1:A:37:SER:HB3	1:A:40:GLU:HG3	1.98	0.45
1:A:145:SER:HB3	1:A:177:PHE:CE1	2.51	0.45
1:A:1:MET:O	1:A:2:ASP:HB3	2.17	0.45
1:A:92:ASP:O	1:A:96:ASP:HB2	2.16	0.45
1:A:119:LEU:HD13	1:A:155:ILE:HD12	1.98	0.45
1:B:27:LYS:HA	1:B:100:LEU:HD21	1.98	0.45
1:A:101:LEU:HD12	1:A:101:LEU:HA	1.75	0.44
1:A:211:TYR:CD1	1:A:211:TYR:C	2.90	0.44
1:A:101:LEU:HD21	1:A:121:MET:CB	2.47	0.44
1:A:101:LEU:HD21	1:A:121:MET:CG	2.44	0.44
1:B:171:ALA:O	1:B:175:SER:HB2	2.18	0.44
1:B:1:MET:O	1:B:2:ASP:HB3	2.17	0.44
1:B:211:TYR:CD1	1:B:211:TYR:C	2.90	0.44
1:A:30:THR:HG22	1:A:36:LEU:HD21	2.00	0.44
2:P:2:LEU:HG	2:P:3:ASP:N	2.31	0.44
1:A:142:VAL:HG23	1:A:181:ILE:CG2	2.48	0.44
1:A:119:LEU:HD22	1:A:151:GLU:HB3	1.99	0.44
1:B:45:SER:OG	1:B:117:PHE:HZ	2.01	0.44
1:A:171:ALA:O	1:A:175:SER:HB2	2.18	0.44
1:A:211:TYR:HD1	1:A:211:TYR:C	2.21	0.44
1:B:142:VAL:HG23	1:B:181:ILE:CG2	2.48	0.44
1:B:119:LEU:HD22	1:B:151:GLU:HB3	1.98	0.44
1:A:46:VAL:HG13	1:A:47:ALA:N	2.33	0.44
1:B:119:LEU:HD13	1:B:155:ILE:HD12	1.98	0.44
1:B:46:VAL:HG13	1:B:47:ALA:N	2.33	0.44
1:A:59:TRP:CE2	1:A:132:VAL:HG22	2.52	0.44
1:B:169:GLY:HA3	2:Q:2:LEU:CD1	2.46	0.43
1:B:116:VAL:HA	1:B:152:ALA:CB	2.47	0.43
1:B:59:TRP:CE2	1:B:132:VAL:HG22	2.52	0.43
1:B:101:LEU:HD21	1:B:121:MET:CB	2.47	0.43
1:A:174:PHE:CD1	1:A:174:PHE:O	2.72	0.43
1:B:33:GLY:O	1:B:34:ALA:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:O	1:B:100:LEU:CD1	2.67	0.43
1:B:30:THR:HG22	1:B:36:LEU:HD21	2.00	0.43
1:A:12:LEU:HG	1:B:82:TYR:HD2	1.82	0.43
1:B:142:VAL:O	1:B:177:PHE:HZ	2.02	0.43
1:A:142:VAL:O	1:A:177:PHE:HZ	2.02	0.43
1:A:178:TYR:O	1:A:183:ASN:N	2.52	0.43
1:A:96:ASP:O	1:A:100:LEU:CD1	2.67	0.43
1:B:211:TYR:HD1	1:B:211:TYR:C	2.21	0.42
1:A:220:LEU:H	1:A:220:LEU:HD13	1.85	0.42
1:B:119:LEU:CD2	1:B:151:GLU:HB3	2.49	0.42
1:A:119:LEU:CD2	1:A:151:GLU:HB3	2.49	0.42
1:B:174:PHE:CD1	1:B:174:PHE:O	2.72	0.42
1:A:196:PHE:O	1:A:199:ALA:HB3	2.19	0.42
1:B:196:PHE:O	1:B:199:ALA:HB3	2.19	0.42
1:A:174:PHE:HD1	1:A:174:PHE:O	2.02	0.42
1:B:85:LYS:O	1:B:89:GLU:HG3	2.20	0.42
1:A:46:VAL:CG1	1:A:47:ALA:N	2.83	0.42
1:B:221:LEU:O	1:B:225:LEU:HD13	2.20	0.42
1:B:174:PHE:HD1	1:B:174:PHE:O	2.02	0.42
1:A:162:PRO:C	1:A:164:HIS:N	2.72	0.42
1:A:162:PRO:HG3	1:A:167:ARG:CZ	2.50	0.42
1:B:162:PRO:HG3	1:B:167:ARG:CZ	2.50	0.42
1:B:179:TYR:CD1	1:B:179:TYR:C	2.93	0.42
1:B:220:LEU:HD13	1:B:220:LEU:H	1.85	0.42
1:A:33:GLY:O	1:A:34:ALA:O	2.37	0.42
1:A:164:HIS:HA	1:A:165:PRO:HD2	1.76	0.42
1:A:221:LEU:O	1:A:225:LEU:HD13	2.20	0.42
1:B:165:PRO:CB	1:B:217:ILE:HD11	2.50	0.42
1:B:126:TYR:HD1	1:B:141:ILE:HG23	1.85	0.42
1:B:46:VAL:CG1	1:B:47:ALA:N	2.83	0.41
1:A:165:PRO:CB	1:A:217:ILE:HD11	2.50	0.41
1:B:178:TYR:O	1:B:183:ASN:N	2.52	0.41
1:A:126:TYR:HD1	1:A:141:ILE:HG23	1.85	0.41
1:A:45:SER:OG	1:A:117:PHE:HZ	2.01	0.41
1:A:179:TYR:C	1:A:179:TYR:CD1	2.93	0.41
1:A:221:LEU:O	1:A:225:LEU:CD1	2.68	0.41
1:B:221:LEU:O	1:B:225:LEU:CD1	2.68	0.41
1:B:219:GLN:O	1:B:222:ARG:HB3	2.21	0.41
1:A:85:LYS:O	1:A:89:GLU:HG3	2.20	0.41
1:B:162:PRO:C	1:B:164:HIS:N	2.72	0.41
1:B:210:SER:O	1:B:211:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:O	1:A:211:TYR:HB2	2.21	0.41
1:A:12:LEU:HG	1:B:82:TYR:CD2	2.56	0.41
1:A:165:PRO:HB3	1:A:217:ILE:CD1	2.51	0.41
1:B:165:PRO:HB3	1:B:217:ILE:CD1	2.51	0.41
1:B:127:ARG:O	1:B:130:ALA:HB3	2.21	0.41
1:B:38:ASN:O	1:B:41:ARG:HB3	2.21	0.41
1:A:120:LYS:HB3	1:A:120:LYS:HE2	1.94	0.41
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.93	0.40
1:A:225:LEU:N	1:A:225:LEU:HD12	2.37	0.40
1:A:27:LYS:HA	1:A:100:LEU:CD2	2.51	0.40
1:B:101:LEU:HA	1:B:101:LEU:HD12	1.76	0.40
1:B:31:GLU:HA	1:B:104:PHE:CE2	2.57	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	210/245 (86%)	152 (72%)	48 (23%)	10 (5%)	3	23
1	B	210/245 (86%)	152 (72%)	48 (23%)	10 (5%)	3	23
2	P	3/20 (15%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/20 (15%)	2 (67%)	1 (33%)	0	100	100
All	All	426/530 (80%)	308 (72%)	98 (23%)	20 (5%)	3	23

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
1	A	166	ILE
1	A	211	TYR

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Mol	Chain	Res	Type
1	B	34	ALA
1	B	166	ILE
1	B	211	TYR
1	A	201	ALA
1	A	212	LYS
1	B	201	ALA
1	B	212	LYS
1	A	17	GLU
1	A	35	GLU
1	B	17	GLU
1	B	35	GLU
1	A	113	GLU
1	A	163	THR
1	A	197	ASP
1	B	113	GLU
1	B	163	THR
1	B	197	ASP

### 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	187/209 (90%)	157 (84%)	30 (16%)	3	14
1	B	187/209 (90%)	157 (84%)	30 (16%)	3	14
2	P	5/19 (26%)	5 (100%)	0	100	100
2	Q	5/19 (26%)	5 (100%)	0	100	100
All	All	384/456 (84%)	324 (84%)	60 (16%)	3	15

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	MET
1	A	29	VAL
1	A	30	THR

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Mol	Chain	Res	Type
1	A	45	SER
1	A	49	LYS
1	A	78	MET
1	A	81	GLU
1	A	82	TYR
1	A	90	LEU
1	A	96	ASP
1	A	98	LEU
1	A	101	LEU
1	A	105	LEU
1	A	110	SER
1	A	114	SER
1	A	119	LEU
1	A	136	ASP
1	A	150	GLN
1	A	160	MET
1	A	168	LEU
1	A	179	TYR
1	A	183	ASN
1	A	191	LEU
1	A	211	TYR
1	A	213	ASP
1	A	218	MET
1	A	221	LEU
1	A	222	ARG
1	A	223	ASP
1	B	1	MET
1	B	22	MET
1	B	29	VAL
1	B	30	THR
1	B	45	SER
1	B	49	LYS
1	B	78	MET
1	B	81	GLU
1	B	82	TYR
1	B	90	LEU
1	B	96	ASP
1	B	98	LEU
1	B	101	LEU
1	B	105	LEU
1	B	110	SER
1	B	114	SER

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Mol	Chain	Res	Type
1	B	119	LEU
1	B	136	ASP
1	B	150	GLN
1	B	160	MET
1	B	168	LEU
1	B	179	TYR
1	B	183	ASN
1	B	191	LEU
1	B	211	TYR
1	B	213	ASP
1	B	218	MET
1	B	221	LEU
1	B	222	ARG
1	B	223	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	32	GLN
1	A	67	GLN
1	A	76	GLN
1	A	111	GLN
1	A	146	GLN
1	A	164	HIS
1	A	183	ASN
1	B	8	GLN
1	B	32	GLN
1	B	67	GLN
1	B	76	GLN
1	B	111	GLN
1	B	146	GLN
1	B	164	HIS
1	B	183	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	216/245 (88%)	0.89	24 (11%) <b>7</b> <b>7</b>	16, 54, 85, 94	0
1	B	216/245 (88%)	0.83	25 (11%) <b>6</b> <b>6</b>	16, 54, 85, 94	0
2	P	5/20 (25%)	2.17	3 (60%) <b>0</b> <b>0</b>	73, 77, 82, 83	0
2	Q	5/20 (25%)	1.65	2 (40%) <b>0</b> <b>1</b>	73, 77, 82, 83	0
All	All	442/530 (83%)	0.89	54 (12%) <b>5</b> <b>5</b>	16, 54, 85, 94	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	SER	8.1
1	B	112	ALA	6.5
1	B	73	GLU	6.3
1	B	116	VAL	4.8
1	B	184	SER	4.4
1	A	185	PRO	4.3
1	B	38	ASN	3.7
1	A	182	LEU	3.6
1	B	109	ALA	3.6
1	A	73	GLU	3.4
2	Q	4	LEU	3.4
1	B	166	ILE	3.3
2	P	5	GLU	3.3
1	A	76	GLN	3.2
1	B	53	GLY	3.2
2	P	4	LEU	3.2
1	B	212	LYS	3.1
1	B	7	VAL	3.1
1	B	107	PRO	3.1
1	B	1	MET	3.1
1	A	65	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	227	LEU	3.0
1	A	211	TYR	3.0
1	A	181	ILE	2.9
1	A	36	LEU	2.7
1	B	220	LEU	2.7
1	B	211	TYR	2.7
1	A	210	SER	2.6
1	B	161	GLN	2.6
2	Q	1	TRP	2.5
1	B	110	SER	2.5
1	B	44	LEU	2.5
1	B	180	GLU	2.4
1	B	177	PHE	2.4
1	A	177	PHE	2.4
1	A	216	LEU	2.3
1	A	30	THR	2.3
1	B	59	TRP	2.3
1	A	186	GLU	2.3
1	B	22	MET	2.3
1	A	79	ALA	2.3
1	A	166	ILE	2.3
1	A	17	GLU	2.2
1	B	19	TYR	2.2
1	A	213	ASP	2.2
1	B	6	LEU	2.2
1	A	132	VAL	2.2
1	B	99	SER	2.1
1	A	3	LYS	2.1
1	B	170	LEU	2.1
1	A	148	ALA	2.1
2	P	1	TRP	2.0
1	A	45	SER	2.0
1	A	95	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.