



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:03 PM UTC

PDB ID : 1A38 / pdb_00001a38
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

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

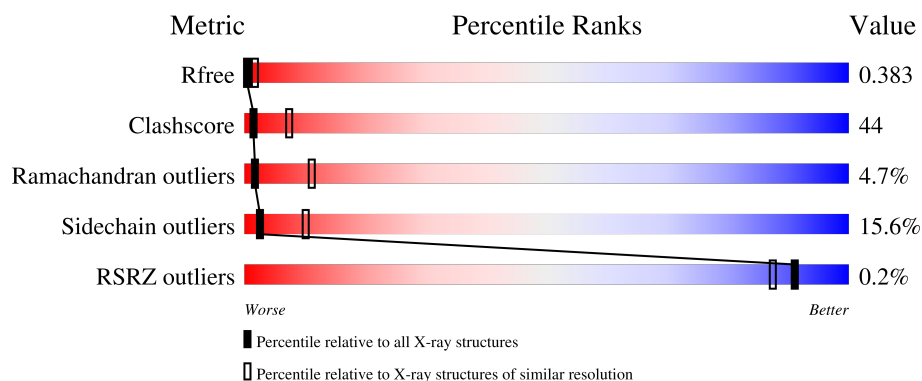
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	245	24% 44% 18% • 12%
1	B	245	23% 46% 18% • 12%
2	P	20	5% 20% 75%
2	Q	20	5% 20% 75%

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			

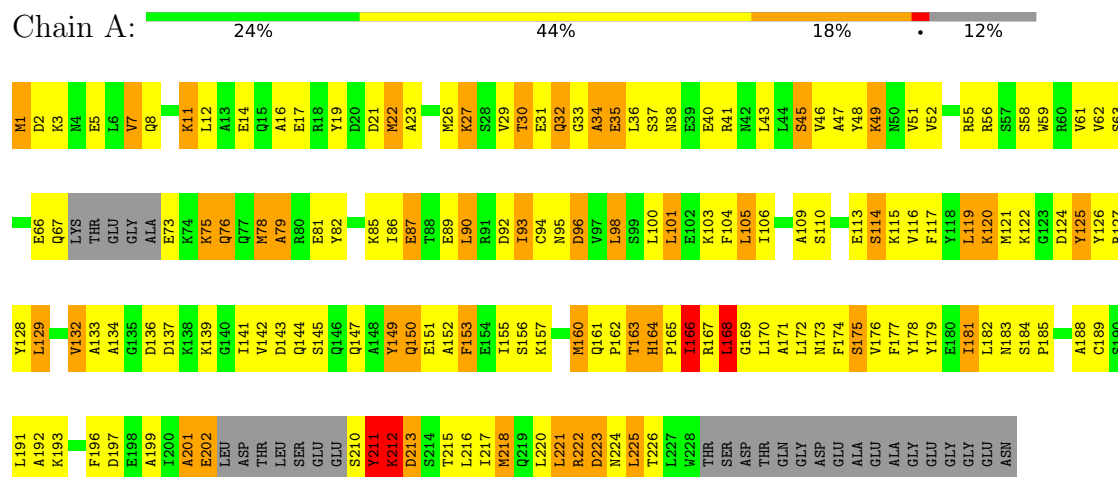
- Molecule 2 is a protein called R18 PEPTIDE (PHCVPRDLSWLDLEANMCLP).

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			

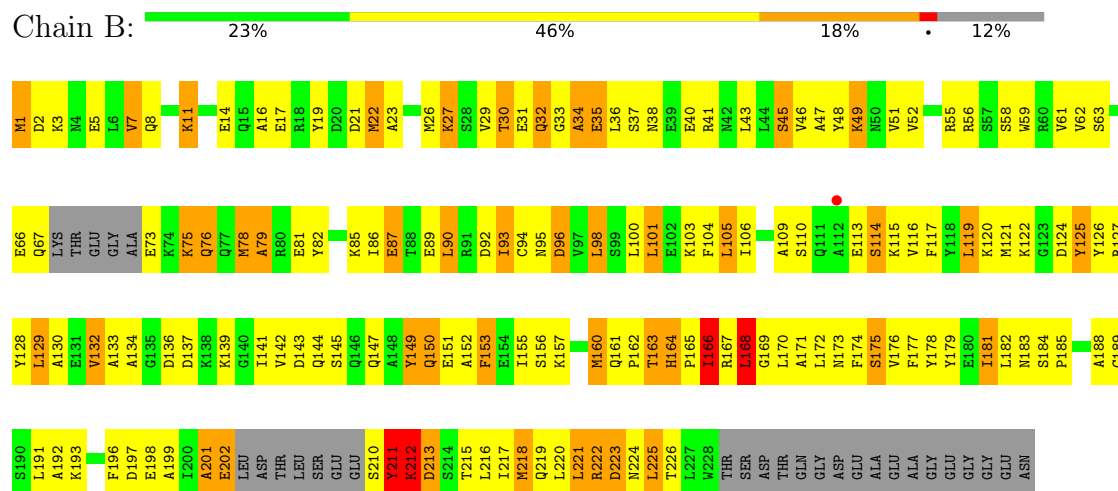
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 14-3-3 PROTEIN ZETA



• Molecule 1: 14-3-3 PROTEIN ZETA



• Molecule 2: R18 PEPTIDE (PHCVPRDLSWLDLEANMCLP)



- Molecule 2: R18 PEPTIDE (PHCVPRDLSWLDLEANMCLP)

Chain Q:  5% 20% 75%

PHE	HIS	CYS	VAL	PRO	ARG	ASP	LEU	SER	W1	L2	D3	L4	ES	ALA	ASN	MET	CYS	LEU	PRO
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	95.52Å 95.52Å 235.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.35 20.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-3.35) 97.0 (20.00-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 3.11Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.330 , 0.390 0.368 , 0.383	Depositor DCC
R_{free} test set	2087 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 121.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.449 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	3554	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.65	0/1751	1.41	37/2348 (1.6%)
1	B	0.65	0/1751	1.42	37/2348 (1.6%)
2	P	0.75	0/48	1.01	0/65
2	Q	0.75	0/48	1.01	0/65
All	All	0.65	0/3598	1.41	74/4826 (1.5%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	TYR	N-CA-C	10.39	125.34	112.87
1	A	19	TYR	N-CA-C	10.37	125.32	112.87
1	A	161	GLN	N-CA-C	9.31	123.51	110.01
1	B	161	GLN	N-CA-C	9.29	123.48	110.01
1	A	153	PHE	N-CA-C	-9.08	100.22	111.11
1	B	153	PHE	N-CA-C	-9.07	100.23	111.11
1	A	133	ALA	N-CA-C	8.77	121.65	110.33
1	B	133	ALA	N-CA-C	8.77	121.64	110.33
1	B	120	LYS	N-CA-C	-8.35	100.47	111.24
1	A	120	LYS	N-CA-C	-8.33	100.49	111.24
1	B	7	VAL	N-CA-C	-8.24	102.78	110.53
1	A	7	VAL	N-CA-C	-8.20	102.82	110.53
1	A	27	LYS	N-CA-C	-7.88	102.69	111.28
1	B	134	ALA	N-CA-C	7.86	122.65	112.12
1	B	27	LYS	N-CA-C	-7.85	102.72	111.28
1	A	134	ALA	N-CA-C	7.82	122.60	112.12
1	B	164	HIS	CA-C-N	7.75	129.53	119.84
1	B	164	HIS	C-N-CA	7.75	129.53	119.84
1	A	164	HIS	CA-C-N	7.75	129.53	119.84
1	A	164	HIS	C-N-CA	7.75	129.53	119.84
1	B	137	ASP	N-CA-C	-7.71	102.88	111.28
1	A	137	ASP	N-CA-C	-7.68	102.88	111.71
1	A	168	LEU	N-CA-C	-7.52	102.77	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	LEU	N-CA-C	-7.49	102.81	110.97
1	A	161	GLN	CA-C-N	6.68	126.27	119.19
1	A	161	GLN	C-N-CA	6.68	126.27	119.19
1	B	161	GLN	CA-C-N	6.68	126.27	119.19
1	B	161	GLN	C-N-CA	6.68	126.27	119.19
1	B	93	ILE	CB-CA-C	-6.38	103.67	112.02
1	B	32	GLN	N-CA-C	-6.37	98.97	109.80
1	A	93	ILE	CB-CA-C	-6.36	103.69	112.02
1	A	32	GLN	N-CA-C	-6.36	99.00	109.80
1	A	75	LYS	N-CA-C	-6.35	104.41	111.71
1	A	181	ILE	N-CA-C	6.34	122.53	109.34
1	B	181	ILE	N-CA-C	6.33	122.50	109.34
1	B	75	LYS	N-CA-C	-6.33	104.44	111.71
1	B	125	TYR	N-CA-C	6.20	117.70	111.07
1	B	160	MET	N-CA-C	6.17	118.24	108.79
1	A	125	TYR	N-CA-C	6.17	117.67	111.07
1	A	160	MET	N-CA-C	6.17	118.22	108.79
1	A	76	GLN	N-CA-C	5.92	117.73	111.28
1	B	76	GLN	N-CA-C	5.92	117.73	111.28
1	B	122	LYS	N-CA-C	-5.85	103.89	111.02
1	A	122	LYS	N-CA-C	-5.83	103.90	111.02
1	A	11	LYS	N-CA-C	-5.82	103.74	111.24
1	B	11	LYS	N-CA-C	-5.81	103.74	111.24
1	B	225	LEU	N-CA-C	-5.81	105.69	112.89
1	A	5	GLU	N-CA-C	-5.75	105.37	112.90
1	B	5	GLU	N-CA-C	-5.71	105.42	112.90
1	B	212	LYS	N-CA-C	5.71	122.96	110.80
1	A	212	LYS	N-CA-C	5.71	122.95	110.80
1	B	175	SER	N-CA-C	-5.62	105.07	111.14
1	B	3	LYS	N-CA-C	5.60	118.11	111.33
1	A	3	LYS	N-CA-C	5.59	118.09	111.33
1	B	103	LYS	N-CA-C	5.59	120.26	113.38
1	A	175	SER	N-CA-C	-5.59	105.10	111.14
1	A	103	LYS	N-CA-C	5.58	120.24	113.38
1	A	95	ASN	N-CA-C	-5.32	105.48	111.28
1	B	95	ASN	N-CA-C	-5.31	105.49	111.28
1	A	79	ALA	N-CA-C	-5.30	105.39	111.07
1	B	79	ALA	N-CA-C	-5.30	105.39	111.07
1	B	166	ILE	N-CA-C	-5.25	98.42	109.34
1	B	202	GLU	N-CA-C	5.24	125.67	111.00
1	A	166	ILE	N-CA-C	-5.24	98.44	109.34
1	A	202	GLU	N-CA-C	5.23	125.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	TYR	N-CA-C	-5.22	105.50	111.14
1	B	21	ASP	N-CA-C	-5.21	105.02	111.33
1	A	149	TYR	N-CA-C	-5.21	105.52	111.14
1	A	225	LEU	N-CA-C	-5.20	105.68	112.23
1	A	21	ASP	N-CA-C	-5.18	105.06	111.33
1	B	182	LEU	N-CA-C	5.09	118.59	112.38
1	A	182	LEU	N-CA-C	5.08	118.58	112.38
1	B	193	LYS	N-CA-C	-5.07	105.64	111.07
1	A	193	LYS	N-CA-C	-5.06	105.65	111.07

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	155	0
1	B	1730	0	1726	153	0
2	P	47	0	44	8	0
2	Q	47	0	44	8	0
All	All	3554	0	3540	309	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 44.

All (309) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:Q:1:TRP:CD1	2:Q:2:LEU:H	2.07	0.73
2:P:1:TRP:CD1	2:P:2:LEU:H	2.06	0.72
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
1:A:100:LEU:HD12	1:A:100:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:MET:SD	1:B:47:ALA:HB2	2.38	0.64
1:B:43:LEU:O	1:B:46:VAL:HG12	1.98	0.64
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
1:A:22:MET:SD	1:A:47:ALA:HB2	2.38	0.63
2:P:1:TRP:HD1	2:P:2:LEU:H	1.46	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:A:143:ASP:O	1:A:147:GLN:HG3	2.00	0.62
1:B:101:LEU:HD21	1:B:121:MET:HG2	1.80	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:162:PRO:C	1:B:164:HIS:H	2.07	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:A:59:TRP:HE1	1:A:87:GLU:HG3	1.65	0.61
1:A:101:LEU:HD21	1:A:121:MET:HG2	1.80	0.61
1:B:192:ALA:HB1	1:B:225:LEU:HD11	1.82	0.61
1:A:94:CYS:O	1:A:98:LEU:HB2	2.00	0.61
1:A:162:PRO:C	1:A:164:HIS:H	2.07	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: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
1:A:66:GLU:HB2	1:A:79:ALA:HB1	1.81	0.61
1:A:116:VAL:HA	1:A:152:ALA:HB1	1.83	0.61
1:B:116:VAL:HA	1:B:152:ALA:HB1	1.83	0.61
1:B:35:GLU:HA	1:B:35:GLU:OE1	1.99	0.60
1:A:30:THR:C	1:A:32:GLN:H	2.07	0.60
1:B:30:THR:C	1:B:32:GLN:H	2.07	0.60
1:A:51:VAL:HG13	1:A:55:ARG:NH1	2.17	0.59
1:A:124:ASP:O	1:A:127:ARG:HB3	2.03	0.59
1:A:216:LEU:O	1:A:220:LEU:HD13	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:124:ASP:O	1:B:127:ARG:HB3	2.03	0.59
1:B:192:ALA:CB	1:B:225:LEU:HD11	2.33	0.59
1:B:216:LEU:O	1:B:220:LEU:HD13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:CD	1:B:132:VAL:HG13	2.30	0.57
1:A:8:GLN:NE2	1:B:78:MET:HE3	2.20	0.57
1:A:38:ASN:HA	1:A:41:ARG:HB3	1.87	0.57
1:A:163:THR:HG22	1:A:163:THR:O	2.05	0.57
1:B:87:GLU:HG2	1:B:132:VAL:HG13	1.87	0.57
1:A:87:GLU:CD	1:A:132:VAL:HG13	2.30	0.57
1:B:199:ALA:HB1	1:B:218:MET:HE3	1.86	0.57
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: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:A:199:ALA:HB1	1:A:218:MET:HE3	1.86	0.55
1:A:8:GLN:CD	1:B:75:LYS:HD2	2.31	0.55
1:B:59:TRP:NE1	1:B:87:GLU:HG3	2.22	0.55
1:B:14:GLU:C	1:B:16:ALA:H	2.15	0.54
1:A:8:GLN:HE21	1:B:78:MET:HE3	1.73	0.54
1:A:14:GLU:C	1:A:16:ALA:H	2.15	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:87:GLU:HG2	1:A:132:VAL:CG1	2.40	0.52
1:B:87:GLU:HG2	1:B: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:A:126:TYR:CE1	1:A:144:GLN:HB3	2.45	0.52
1:A:169:GLY:O	1:A:172:LEU:HB3	2.09	0.52
1:B:61:VAL:HG13	1:B:62:VAL:H	1.75	0.52
1:B:87:GLU:CG	1:B:132:VAL:HG13	2.40	0.52
1:A:87:GLU:CG	1:A:132:VAL:HG13	2.40	0.52
1:A:125:TYR:HA	1:A:128:TYR:CD2	2.45	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:199:ALA:CB	1:A:218:MET:HE3	2.42	0.50
1:B:153:PHE:O	1:B:157:LYS:HB2	2.12	0.50
1:B:211:TYR:CD1	1:B:211:TYR:C	2.90	0.50
1:A:178:TYR:HD1	1:A:184:SER:HB3	1.77	0.49
1:A:192:ALA:O	1:A:196:PHE:HB3	2.13	0.49
1:A:211:TYR:CD1	1:A:211:TYR:C	2.90	0.49
1:A:76:GLN:O	1:A:79:ALA:HB3	2.13	0.49
1:B:199:ALA:CB	1:B:218:MET:HE3	2.42	0.49
1:A:152:ALA:HA	1:A:155:ILE:HB	1.94	0.49
1:A:211:TYR:C	1:A:211:TYR:HD1	2.21	0.49
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:63:SER:O	1:B:67:GLN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TYR:HD1	1:B:184:SER:HB3	1.77	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:A:153:PHE:O	1:A:157:LYS:HB2	2.12	0.48
1:B:213:ASP:HA	1:B:216:LEU:HD12	1.96	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:172:LEU:O	1:B:175:SER:HB3	2.14	0.48
1:B:221:LEU:O	1:B:224:ASN:HB2	2.14	0.48
1:A:63:SER:O	1:A:67:GLN:N	2.45	0.47
1:A:211:TYR:CD1	1:A:212:LYS:N	2.82	0.47
1:B:192:ALA:O	1:B:196:PHE:HB3	2.13	0.47
1:A:23:ALA:HB1	1:A:48:TYR:CE2	2.49	0.47
1:A:117:PHE:HB2	1:A:166:ILE:HD11	1.96	0.47
1:A:213:ASP:HA	1:A:216:LEU:HD12	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:173:ASN:HA	1:A:176:VAL:HG12	1.95	0.47
1:A:221:LEU:O	1:A:224:ASN:HB2	2.14	0.47
1:B:220:LEU:H	1:B:220:LEU:CD1	2.27	0.47
1:A:172:LEU:O	1:A:175:SER:HB3	2.14	0.47
1:B:117:PHE:HB2	1:B:166:ILE:HD11	1.96	0.47
1:B:211:TYR:C	1:B:211:TYR:HD1	2.21	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
1:B:179:TYR:CD1	1:B:179:TYR:C	2.93	0.47
1:A:162:PRO:C	1:A:164:HIS:N	2.72	0.47
2:Q:1:TRP:CD1	2:Q:2:LEU:N	2.80	0.46
1:A:220:LEU:CD1	1:A:220:LEU:N	2.78	0.46
1:B:220:LEU:CD1	1:B:220:LEU:N	2.78	0.46
1:A:26:MET:HE1	1:A:40:GLU:HB3	1.97	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:B:26:MET:HE1	1:B:40:GLU:HB3	1.97	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
1:A:179:TYR:CD1	1:A:179:TYR:C	2.93	0.45
1:B:145:SER:HB3	1:B:177:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MET:HE3	1:B:8:GLN:NE2	2.32	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:37:SER:HB3	1:B:40:GLU:HG3	1.98	0.45
1:B:82:TYR:O	1:B:86:ILE:HG13	2.16	0.45
1:B:92:ASP:O	1:B:96:ASP:HB2	2.17	0.45
1:A:37:SER:HB3	1:A:40:GLU:HG3	1.98	0.45
1:B:101:LEU:HD21	1:B:121:MET:CG	2.44	0.45
1:A:1:MET:O	1:A:2:ASP:HB3	2.17	0.45
1:A:145:SER:HB3	1:A:177:PHE:CE1	2.51	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
2:Q:2:LEU:HG	2:Q:3:ASP:N	2.31	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: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:1:MET:O	1:B:2:ASP:HB3	2.17	0.44
1:B:171:ALA:O	1:B:175:SER:HB2	2.18	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:A:171:ALA:O	1:A:175:SER:HB2	2.18	0.44
1:B:45:SER:OG	1:B:117:PHE:HZ	2.01	0.44
1:A:46:VAL:HG13	1:A:47:ALA:N	2.33	0.44
1:B:119:LEU:HD22	1:B:151:GLU:HB3	1.98	0.44
1:B:142:VAL:HG23	1:B:181:ILE:CG2	2.48	0.44
1:B:119:LEU:HD13	1:B:155:ILE:HD12	1.98	0.44
1:A:59:TRP:CE2	1:A:132:VAL:HG22	2.52	0.44
1:B:46:VAL:HG13	1:B:47:ALA:N	2.33	0.44
1:B:169:GLY:HA3	2:Q:2:LEU:CD1	2.46	0.43
1:B:59:TRP:CE2	1:B:132:VAL:HG22	2.52	0.43
1:B:116:VAL:HA	1:B:152:ALA:CB	2.47	0.43
1:B:101:LEU:HD21	1:B:121:MET:CB	2.47	0.43
1:A:174:PHE:O	1:A:174:PHE:CD1	2.72	0.43
1:B:33:GLY:O	1:B:34:ALA:O	2.37	0.43
1:A:12:LEU:HG	1:B:82:TYR:HD2	1.82	0.43
1:B:30:THR:HG22	1:B:36:LEU:HD21	2.00	0.43
1:B:96:ASP:O	1:B:100:LEU:CD1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:O	1:A:177:PHE:HZ	2.02	0.43
1:B:142:VAL:O	1:B:177:PHE:HZ	2.02	0.43
1:A:96:ASP:O	1:A:100:LEU:CD1	2.67	0.43
1:A:178:TYR:O	1:A:183:ASN:N	2.52	0.43
1:A:119:LEU:CD2	1:A:151:GLU:HB3	2.49	0.42
1:A:220:LEU:HD13	1:A:220:LEU:H	1.85	0.42
1:B:119:LEU:CD2	1:B:151:GLU:HB3	2.49	0.42
1:B:174:PHE:CD1	1:B:174:PHE:O	2.72	0.42
1:A:14:GLU:C	1:A:16:ALA:N	2.77	0.42
1:A:174:PHE:O	1:A:174:PHE:HD1	2.02	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:46:VAL:CG1	1:A:47:ALA:N	2.83	0.42
1:B:85:LYS:O	1:B:89:GLU:HG3	2.20	0.42
1:B:174:PHE:O	1:B:174:PHE:HD1	2.02	0.42
1:B:221:LEU:O	1:B:225:LEU:HD13	2.20	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:A:33:GLY:O	1:A:34:ALA:O	2.37	0.42
1:B:105:LEU:O	1:B:106:ILE:C	2.61	0.42
1:B:220:LEU:HD13	1:B:220:LEU:H	1.85	0.42
1:A:30:THR:C	1:A:32:GLN:N	2.76	0.42
1:A:105:LEU:O	1:A:106:ILE:C	2.61	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:126:TYR:HD1	1:B:141:ILE:HG23	1.85	0.42
1:B:165:PRO:CB	1:B:217:ILE:HD11	2.50	0.42
1:A:117:PHE:CD1	1:A:117:PHE:C	2.98	0.41
1:A:165:PRO:CB	1:A:217:ILE:HD11	2.50	0.41
1:B:117:PHE:CD1	1:B:117:PHE:C	2.98	0.41
1:B:178:TYR:O	1:B:183:ASN:N	2.52	0.41
1:B:46:VAL:CG1	1:B:47:ALA:N	2.83	0.41
1:A:45:SER:OG	1:A:117:PHE:HZ	2.01	0.41
1:A:126:TYR:HD1	1:A:141:ILE:HG23	1.85	0.41
1:B:14:GLU:C	1:B:16:ALA:N	2.77	0.41
1:B:162:PRO:C	1:B:164:HIS:N	2.72	0.41
1:A:221:LEU:O	1:A:225:LEU:CD1	2.68	0.41
1:A:222:ARG:C	1:A:224:ASN:N	2.77	0.41
1:B:219:GLN:O	1:B:222:ARG:HB3	2.21	0.41
1:B:221:LEU:O	1:B:225:LEU:CD1	2.68	0.41
1:A:85:LYS:O	1:A:89:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HG	1:B:82:TYR:CD2	2.56	0.41
1:A:179:TYR:C	1:A:179:TYR:HD1	2.29	0.41
1:A:210:SER:O	1:A:211:TYR:HB2	2.21	0.41
1:B:210:SER:O	1:B:211:TYR:HB2	2.21	0.41
1:A:120:LYS:HE2	1:A:120:LYS:HB3	1.94	0.41
1:A:165:PRO:HB3	1:A:217:ILE:CD1	2.51	0.41
1:B:38:ASN:O	1:B:41:ARG:HB3	2.21	0.41
1:B:127:ARG:O	1:B:130:ALA:HB3	2.21	0.41
1:B:165:PRO:HB3	1:B:217:ILE:CD1	2.51	0.41
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.93	0.40
1:A:27:LYS:HA	1:A:100:LEU:CD2	2.51	0.40
1:A:225:LEU:HD12	1:A:225:LEU:N	2.37	0.40
1:B:101:LEU:HD12	1:B:101:LEU:HA	1.76	0.40
1:B:31:GLU:HA	1:B:104:PHE:CE2	2.57	0.40
1:B:198:GLU:O	1:B:199:ALA:C	2.64	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%)	2	11
1	B	210/245 (86%)	152 (72%)	48 (23%)	10 (5%)	2	11
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%)	2	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
1	A	166	ILE
1	A	211	TYR
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%)	2	10
1	B	187/209 (90%)	157 (84%)	30 (16%)	2	10
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%)	2	10

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	MET

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Mol	Chain	Res	Type
1	A	29	VAL
1	A	30	THR
1	A	45	SER
1	A	49	LYS
1	A	78	MET
1	A	81	GLU
1	A	87	GLU
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	129	LEU
1	A	132	VAL
1	A	136	ASP
1	A	150	GLN
1	A	160	MET
1	A	168	LEU
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	87	GLU
1	B	90	LEU
1	B	96	ASP
1	B	98	LEU
1	B	101	LEU
1	B	105	LEU

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Mol	Chain	Res	Type
1	B	110	SER
1	B	114	SER
1	B	119	LEU
1	B	129	LEU
1	B	132	VAL
1	B	136	ASP
1	B	150	GLN
1	B	160	MET
1	B	168	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	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

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	216/245 (88%)	-0.50	0 100 100	16, 54, 85, 94	0
1	B	216/245 (88%)	-0.49	1 (0%) 87 78	16, 54, 85, 94	0
2	P	5/20 (25%)	0.06	0 100 100	73, 77, 82, 83	0
2	Q	5/20 (25%)	0.21	0 100 100	73, 77, 82, 83	0
All	All	442/530 (83%)	-0.48	1 (0%) 91 87	16, 54, 85, 94	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ALA	3.4

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.