



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:26 AM UTC

PDB ID : 1UIU / pdb_00001uiu
Title : Crystal structures of the liganded and unliganded nickel binding protein NikA from Escherichia coli (Nickel unliganded form)
Authors : Heddle, J.; Scott, D.J.; Unzai, S.; Park, S.-Y.; Tame, J.R.H.
Deposited on : 2003-07-22
Resolution : 1.85 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

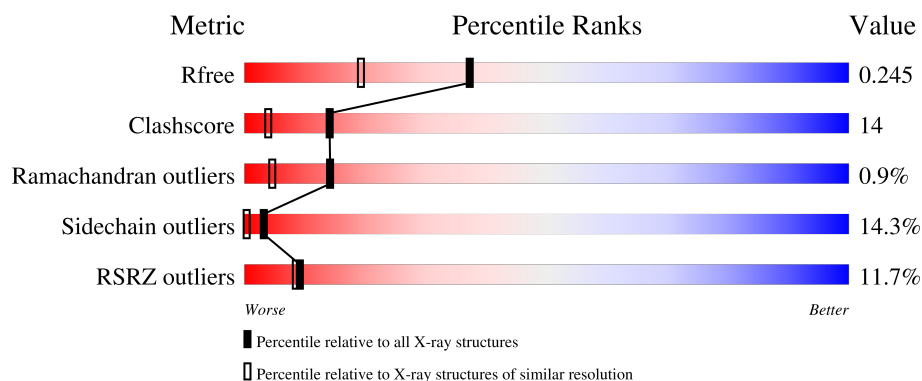
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	502	2% 69% 23% 6% ..
1	B	502	21% 64% 27% 6% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8427 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 Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3941	2525	667	739	10			
1	B	496	Total	C	N	O	S	0	0	0
			3941	2525	667	739	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	ARG	GLN	engineered mutation	UNP P33590
B	1361	ARG	GLN	engineered mutation	UNP P33590

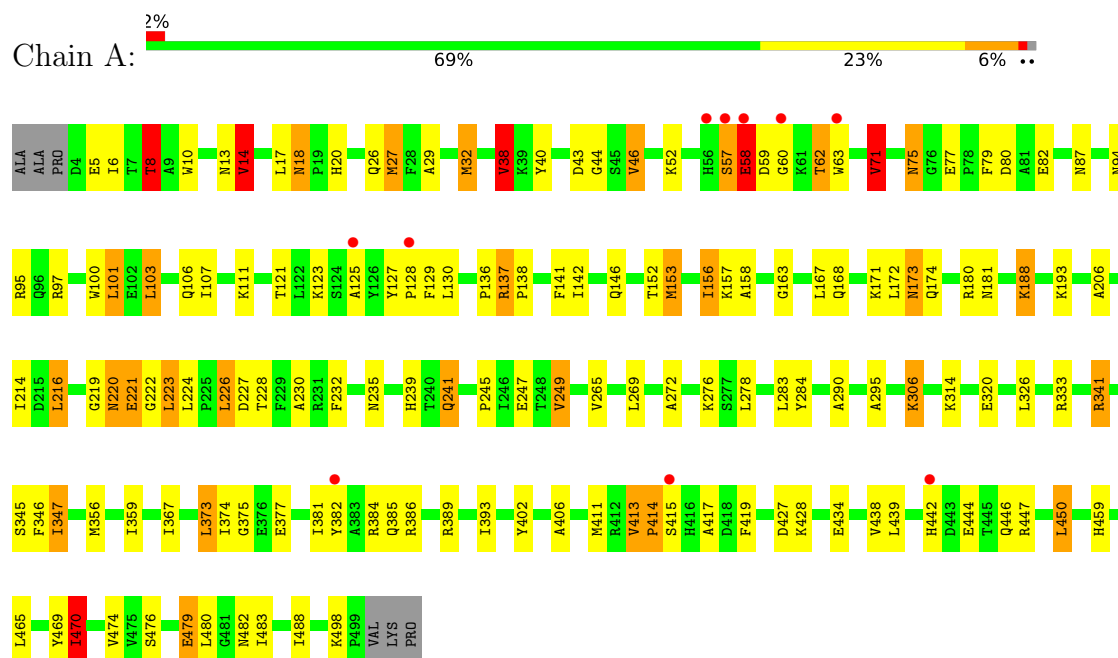
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	350	Total	O	0	0
			350	350		
2	B	195	Total	O	0	0
			195	195		

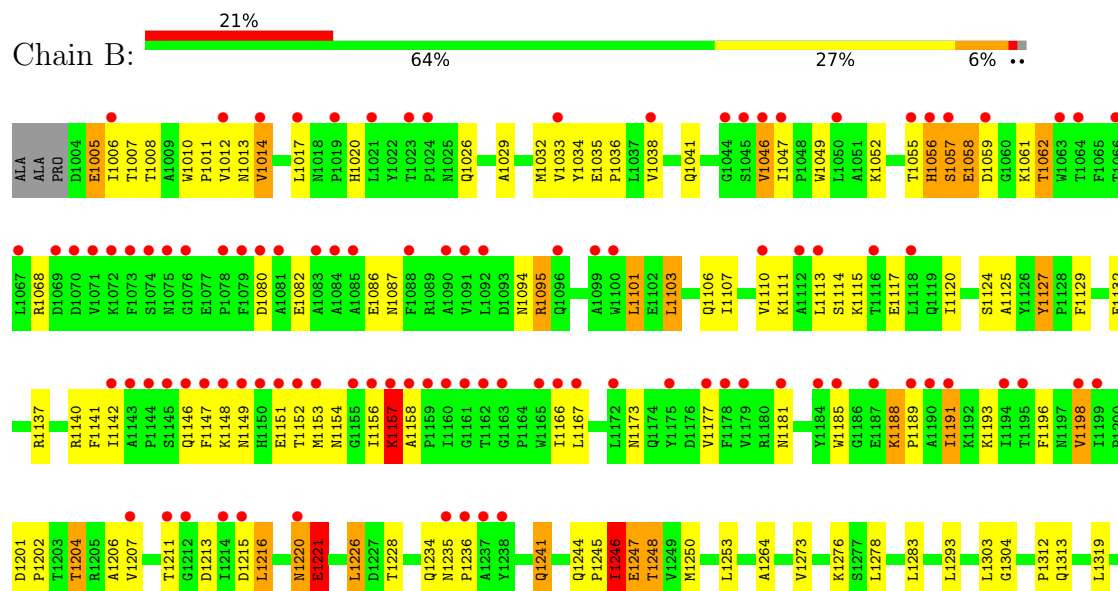
3 Residue-property plots

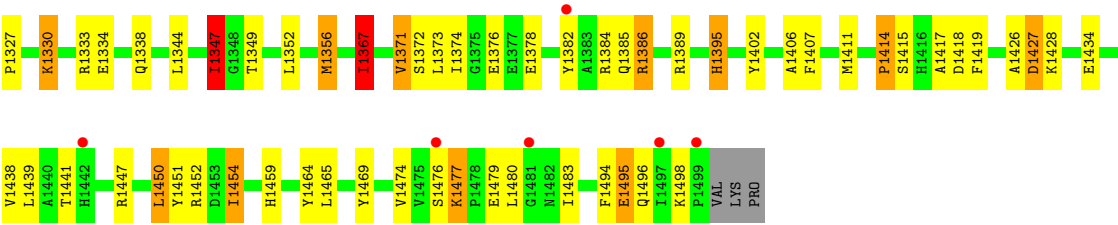
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nickel-binding periplasmic protein



• Molecule 1: Nickel-binding periplasmic protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	126.87Å 126.87Å 60.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 1.85 19.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.85) 87.7 (19.96-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.198 , 0.247 0.200 , 0.245	Depositor DCC
R_{free} test set	4107 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.043 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8427	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	1.27	9/4044 (0.2%)	1.27	23/5508 (0.4%)
1	B	1.11	9/4044 (0.2%)	1.23	24/5508 (0.4%)
All	All	1.19	18/8088 (0.2%)	1.25	47/11016 (0.4%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	MET	SD-CE	-15.57	1.40	1.79
1	B	1356	MET	SD-CE	-13.43	1.46	1.79
1	A	356	MET	SD-CE	-13.26	1.46	1.79
1	A	411	MET	SD-CE	-11.16	1.51	1.79
1	B	1246	ILE	CA-CB	7.95	1.64	1.54
1	B	1427	ASP	CB-CG	-7.81	1.32	1.52
1	B	1427	ASP	CA-CB	7.25	1.66	1.53
1	B	1264	ALA	CA-CB	6.68	1.63	1.53
1	B	1347	ILE	CA-CB	6.62	1.61	1.53
1	B	1372	SER	CA-C	-6.29	1.45	1.52
1	A	27	MET	SD-CE	-5.68	1.65	1.79
1	A	295	ALA	CA-CB	5.51	1.61	1.53
1	A	230	ALA	CA-CB	5.39	1.61	1.53
1	B	1428	LYS	CA-C	5.37	1.59	1.52
1	A	249	VAL	CA-CB	5.32	1.60	1.54
1	A	359	ILE	CA-C	5.24	1.59	1.52
1	B	1333	ARG	NE-CZ	-5.21	1.27	1.33
1	A	428	LYS	C-O	-5.19	1.19	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1303	LEU	CA-C-N	-12.94	96.06	121.41
1	B	1303	LEU	C-N-CA	-12.94	96.06	121.41
1	B	1427	ASP	N-CA-C	9.42	124.32	113.01
1	A	413	VAL	N-CA-C	9.15	117.00	107.76
1	B	1427	ASP	CA-CB-CG	-8.74	103.86	112.60
1	B	1367	ILE	N-CA-CB	-8.21	101.67	112.26
1	B	1427	ASP	CB-CG-OD1	-8.21	99.53	118.40
1	B	1414	PRO	CA-C-N	-7.93	110.06	122.67
1	B	1414	PRO	C-N-CA	-7.93	110.06	122.67
1	A	470	ILE	CG1-CB-CG2	-7.85	87.16	110.70
1	A	414	PRO	CA-C-N	-7.75	109.79	122.65
1	A	414	PRO	C-N-CA	-7.75	109.79	122.65
1	B	1427	ASP	CB-CG-OD2	7.63	135.96	118.40
1	A	8	THR	CB-CA-C	-6.73	98.92	114.41
1	B	1303	LEU	O-C-N	-6.36	113.61	122.76
1	A	71	VAL	N-CA-C	6.32	117.23	108.89
1	A	14	VAL	CG1-CB-CG2	6.21	124.47	110.80
1	A	38	VAL	N-CA-CB	-6.20	102.82	111.19
1	A	153	MET	CG-SD-CE	-6.18	87.31	100.90
1	A	224	LEU	N-CA-C	-6.10	102.73	108.22
1	B	1347	ILE	CB-CA-C	6.10	118.00	111.35
1	B	1141	PHE	N-CA-C	5.91	118.37	108.73
1	A	223	LEU	N-CA-C	5.87	117.35	111.07
1	B	1220	ASN	CA-C-N	5.86	132.72	121.54
1	B	1220	ASN	C-N-CA	5.86	132.72	121.54
1	B	1058	GLU	N-CA-C	5.85	123.25	110.80
1	A	18	ASN	N-CA-C	-5.79	100.85	109.42
1	A	163	GLY	N-CA-C	5.56	118.67	112.00
1	A	346	PHE	CA-C-N	-5.55	114.03	121.80
1	A	346	PHE	C-N-CA	-5.55	114.03	121.80
1	A	173	ASN	N-CA-C	5.46	119.53	112.86
1	B	1247	GLU	CA-C-N	-5.38	115.12	122.93
1	B	1247	GLU	C-N-CA	-5.38	115.12	122.93
1	A	375	GLY	N-CA-C	-5.35	102.52	110.71
1	B	1303	LEU	N-CA-C	-5.32	102.29	109.95
1	A	232	PHE	N-CA-C	-5.30	105.50	111.28
1	A	58	GLU	N-CA-C	-5.24	105.48	111.14
1	A	14	VAL	N-CA-CB	-5.20	100.49	110.78
1	B	1426	ALA	CA-C-N	5.18	131.43	121.18
1	B	1426	ALA	C-N-CA	5.18	131.43	121.18
1	B	1427	ASP	N-CA-CB	-5.18	101.33	110.39
1	A	38	VAL	N-CA-C	-5.16	101.45	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1371	VAL	N-CA-CB	5.13	118.22	111.25
1	A	141	PHE	N-CA-C	5.12	116.76	108.41
1	B	1185	TRP	N-CA-C	5.12	117.76	111.82
1	A	427	ASP	N-CA-C	5.04	118.57	112.93
1	B	1211	THR	N-CA-C	-5.00	107.15	113.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	384	ARG	Sidechain

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	3941	0	3891	109	0
1	B	3941	0	3891	115	0
2	A	350	0	0	11	0
2	B	195	0	0	3	0
All	All	8427	0	7782	224	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 14.

All (224) 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:B:1273:VAL:HG22	2:B:16:HOH:O	1.50	1.08
1:B:1438:VAL:HG12	1:B:1450:LEU:HB3	1.36	1.05
1:B:1438:VAL:CG1	1:B:1450:LEU:HB3	1.86	1.05
1:A:29:ALA:HA	1:A:32:MET:HE2	1.35	1.03
1:A:106:GLN:HE21	1:A:123:LYS:HB2	1.25	0.99
1:B:1029:ALA:HA	1:B:1032:MET:HE2	1.45	0.97
1:B:1082:GLU:O	1:B:1086:GLU:HG2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASN:ND2	1:A:222:GLY:H	1.65	0.94
1:A:153:MET:HE3	2:A:660:HOH:O	1.69	0.93
1:A:29:ALA:HA	1:A:32:MET:CE	1.97	0.93
1:B:1438:VAL:HG12	1:B:1450:LEU:CB	1.98	0.92
1:A:13:ASN:HD21	1:A:173:ASN:H	1.12	0.92
1:A:121:THR:HG23	2:A:793:HOH:O	1.71	0.90
1:A:314:LYS:HE2	2:A:527:HOH:O	1.73	0.88
1:B:1312:PRO:HA	1:B:1367:ILE:HD11	1.55	0.88
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.21	0.86
1:A:106:GLN:NE2	1:A:123:LYS:HB2	1.93	0.84
1:A:58:GLU:HB2	1:A:62:THR:HG23	1.58	0.83
1:B:1347:ILE:HD11	1:B:1349:THR:OG1	1.78	0.82
1:B:1220:ASN:HB3	1:B:1221:GLU:HG3	1.63	0.81
1:A:27:MET:HE1	2:A:590:HOH:O	1.82	0.78
1:B:1451:TYR:HA	1:B:1454:ILE:HD11	1.66	0.76
1:A:125:ALA:HB1	1:A:442:HIS:NE2	2.00	0.76
1:A:220:ASN:HD22	1:A:222:GLY:H	1.34	0.76
1:A:87:ASN:HD21	1:A:142:ILE:H	1.34	0.76
1:A:146:GLN:HE21	1:A:158:ALA:H	1.31	0.76
1:A:434:GLU:O	1:A:438:VAL:HG13	1.86	0.75
1:B:1407:PHE:CE1	1:B:1411:MET:HE3	2.21	0.75
1:A:137:ARG:HD2	2:A:713:HOH:O	1.86	0.75
1:A:180:ARG:HD2	1:A:188:LYS:HG3	1.70	0.72
1:A:94:ASN:ND2	1:A:97:ARG:HG3	2.04	0.72
1:A:57:SER:HB2	1:A:60:GLY:HA2	1.72	0.71
1:A:13:ASN:HD21	1:A:173:ASN:N	1.88	0.71
1:A:220:ASN:HD22	1:A:221:GLU:N	1.89	0.70
1:B:1407:PHE:CE1	1:B:1411:MET:CE	2.74	0.70
1:B:1166:ILE:HD11	1:B:1181:ASN:HD22	1.55	0.70
1:A:171:LYS:HD3	1:A:174:GLN:NE2	2.06	0.69
1:B:1395:HIS:HE1	1:B:1418:ASP:OD2	1.75	0.69
1:A:385:GLN:HB3	1:A:417:ALA:HB2	1.75	0.69
1:B:1376:GLU:OE1	1:B:1384:ARG:NH1	2.26	0.69
1:A:13:ASN:ND2	1:A:173:ASN:H	1.89	0.68
1:A:121:THR:HB	2:A:774:HOH:O	1.92	0.68
1:B:1005:GLU:HB3	1:B:1193:LYS:HB3	1.77	0.67
1:A:8:THR:HG23	1:A:216:LEU:HB3	1.74	0.67
1:B:1313:GLN:CD	1:B:1313:GLN:H	2.03	0.67
1:A:220:ASN:HD22	1:A:220:ASN:C	2.03	0.67
1:A:438:VAL:HG12	1:A:450:LEU:HG	1.77	0.67
1:B:1278:LEU:HD21	1:B:1356:MET:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:HD21	1:A:97:ARG:HG3	1.61	0.66
1:A:239:HIS:HE1	1:A:241:GLN:OE1	1.79	0.65
1:B:1038:VAL:CG2	1:B:1046:VAL:HG13	2.27	0.65
1:A:438:VAL:HG12	1:A:450:LEU:HB3	1.77	0.65
1:B:1411:MET:HE2	1:B:1464:TYR:OH	1.96	0.65
1:B:1441:THR:HG23	1:B:1447:ARG:HD3	1.76	0.65
1:A:438:VAL:HG12	1:A:450:LEU:CG	2.26	0.65
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.62	0.65
1:B:1451:TYR:CD2	1:B:1454:ILE:HD11	2.33	0.64
1:B:1407:PHE:HE1	1:B:1411:MET:CE	2.10	0.64
1:B:1414:PRO:HA	1:B:1419:PHE:CD1	2.33	0.63
1:A:247:GLU:HB3	1:A:470:ILE:HG13	1.81	0.63
1:A:95:ARG:NH2	1:A:107:ILE:O	2.32	0.63
1:B:1248:THR:HG21	1:B:1293:LEU:O	1.99	0.62
1:B:1010:TRP:CG	1:B:1011:PRO:HD2	2.35	0.62
1:A:414:PRO:HA	1:A:419:PHE:CD1	2.35	0.61
1:A:10:TRP:HE1	1:A:26:GLN:NE2	1.96	0.61
1:A:438:VAL:CG1	1:A:450:LEU:HB3	2.31	0.61
1:B:1166:ILE:HD11	1:B:1181:ASN:ND2	2.16	0.60
1:B:1226:LEU:HD23	1:B:1283:LEU:HA	1.83	0.60
1:A:125:ALA:HB1	1:A:442:HIS:CE1	2.37	0.60
1:A:153:MET:CE	2:A:660:HOH:O	2.39	0.60
1:A:168:GLN:NE2	2:A:658:HOH:O	2.35	0.60
1:B:1215:ASP:HB3	1:B:1480:LEU:HD21	1.84	0.60
1:B:1220:ASN:HD21	1:B:1246:ILE:HD11	1.66	0.59
1:B:1038:VAL:HG22	1:B:1046:VAL:HG13	1.85	0.59
1:B:1241:GLN:HG3	1:B:1474:VAL:HB	1.85	0.59
1:A:8:THR:HG22	1:A:216:LEU:O	2.03	0.58
1:A:438:VAL:HG12	1:A:450:LEU:CB	2.33	0.58
1:B:1220:ASN:HB3	1:B:1221:GLU:CG	2.31	0.58
1:B:1006:ILE:HG21	1:B:1480:LEU:HD11	1.86	0.57
1:A:125:ALA:CB	1:A:442:HIS:NE2	2.67	0.57
1:A:247:GLU:HB3	1:A:470:ILE:CG1	2.35	0.57
1:A:278:LEU:C	1:A:278:LEU:HD23	2.29	0.57
1:B:1304:GLY:H	1:B:1452:ARG:HH22	1.52	0.57
1:B:1451:TYR:HA	1:B:1454:ILE:CD1	2.33	0.57
1:A:103:LEU:HD21	1:A:129:PHE:CD2	2.39	0.57
1:B:1106:GLN:NE2	1:B:1124:SER:OG	2.37	0.57
1:B:1226:LEU:HD22	1:B:1352:LEU:HD21	1.86	0.56
1:B:1248:THR:HB	1:B:1469:TYR:CD1	2.40	0.56
1:B:1327:PRO:HB2	1:B:1330:LYS:HG3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1127:TYR:CE2	1:B:1447:ARG:HD2	2.40	0.56
1:A:87:ASN:ND2	1:A:142:ILE:H	2.03	0.56
1:A:290:ALA:HA	1:A:469:TYR:CE2	2.41	0.56
1:B:1441:THR:CG2	1:B:1447:ARG:HD3	2.34	0.56
1:A:130:LEU:HD12	1:A:130:LEU:H	1.70	0.56
1:B:1451:TYR:HD2	1:B:1454:ILE:HD11	1.69	0.56
1:B:1029:ALA:HA	1:B:1032:MET:CE	2.30	0.56
1:B:1312:PRO:CA	1:B:1367:ILE:HD11	2.33	0.56
1:B:1385:GLN:HB3	1:B:1417:ALA:HB2	1.88	0.55
1:B:1386:ARG:HA	1:B:1415:SER:O	2.07	0.54
1:A:20:HIS:HD2	1:A:152:THR:OG1	1.91	0.54
1:B:1248:THR:HG22	2:B:38:HOH:O	2.05	0.54
1:B:1407:PHE:CD1	1:B:1411:MET:HE3	2.41	0.54
1:A:402:TYR:HB3	1:A:406:ALA:HB3	1.89	0.54
1:B:1395:HIS:CE1	1:B:1418:ASP:OD2	2.58	0.54
1:A:38:VAL:HG13	1:A:46:VAL:CG1	2.37	0.54
1:A:5:GLU:HG2	1:A:193:LYS:HB3	1.88	0.53
1:A:438:VAL:CG1	1:A:450:LEU:HG	2.38	0.53
1:B:1035:GLU:CD	1:B:1049:TRP:HE1	2.17	0.53
1:B:1014:VAL:HG13	1:B:1017:LEU:HD21	1.91	0.53
1:B:1438:VAL:HG11	1:B:1450:LEU:HB3	1.84	0.52
1:B:1245:PRO:HB3	1:B:1469:TYR:HB3	1.91	0.52
1:A:341:ARG:HD3	2:A:615:HOH:O	2.10	0.52
1:B:1438:VAL:O	1:B:1441:THR:HG22	2.08	0.52
1:A:71:VAL:HG22	1:A:79:PHE:HB3	1.91	0.52
1:A:220:ASN:HD22	1:A:222:GLY:N	2.03	0.52
1:B:1038:VAL:HG21	1:B:1046:VAL:CG1	2.40	0.52
1:A:306:LYS:O	1:A:459:HIS:HE1	1.93	0.51
1:A:272:ALA:HB2	1:A:367:ILE:HD13	1.92	0.51
1:A:100:TRP:CZ2	1:A:101:LEU:HG	2.45	0.51
1:B:1041:GLN:HG3	1:B:1047:ILE:HG23	1.91	0.51
1:A:75:ASN:ND2	1:A:77:GLU:H	2.08	0.51
1:A:220:ASN:ND2	1:A:220:ASN:C	2.69	0.50
1:B:1057:SER:HB3	1:B:1062:THR:HG23	1.93	0.50
1:A:14:VAL:HG22	1:A:29:ALA:HB2	1.94	0.50
1:A:127:TYR:N	1:A:128:PRO:CD	2.75	0.50
1:B:1477:LYS:HB2	1:B:1480:LEU:HD23	1.93	0.50
1:B:1450:LEU:O	1:B:1454:ILE:HG12	2.12	0.49
1:B:1101:LEU:HD22	1:B:1132:GLU:OE2	2.12	0.49
1:A:171:LYS:HD3	1:A:174:GLN:CD	2.37	0.49
1:B:1014:VAL:HG22	1:B:1029:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:A:283:LEU:HA	1.95	0.49
1:B:1438:VAL:CG1	1:B:1450:LEU:HG	2.43	0.49
1:A:206:ALA:HB1	1:A:228:THR:HG21	1.95	0.49
1:A:265:VAL:O	1:A:269:LEU:HG	2.12	0.49
1:A:479:GLU:CD	1:A:479:GLU:H	2.22	0.48
1:A:20:HIS:CE1	1:A:87:ASN:HD22	2.30	0.48
1:A:71:VAL:HG22	1:A:79:PHE:CB	2.44	0.48
1:A:38:VAL:HG13	1:A:46:VAL:HG11	1.96	0.48
1:B:1146:GLN:HE21	1:B:1157:LYS:HB3	1.78	0.47
1:A:306:LYS:HE3	1:A:306:LYS:HB2	1.66	0.47
1:B:1188:LYS:HA	1:B:1188:LYS:HD3	1.68	0.47
1:A:94:ASN:HD21	1:A:97:ARG:HH11	1.61	0.47
1:B:1012:VAL:HA	1:B:1198:VAL:HG13	1.96	0.47
1:B:1278:LEU:HD21	1:B:1356:MET:CE	2.43	0.47
1:A:103:LEU:O	1:A:107:ILE:HG13	2.15	0.47
1:B:1201:ASP:HB3	1:B:1204:THR:OG1	2.14	0.47
1:B:1451:TYR:HA	1:B:1454:ILE:CG1	2.45	0.47
1:A:136:PRO:HD3	1:A:488:ILE:HD13	1.97	0.46
1:B:1017:LEU:O	1:B:1034:TYR:OH	2.32	0.46
1:A:14:VAL:HG13	1:A:17:LEU:HD21	1.98	0.46
1:A:220:ASN:HD21	1:A:222:GLY:H	1.54	0.46
1:B:1013:ASN:HD21	1:B:1173:ASN:H	1.62	0.46
1:B:1378:GLU:HG3	1:B:1382:TYR:CE1	2.50	0.46
1:B:1438:VAL:HG12	1:B:1450:LEU:HG	1.97	0.46
1:B:1010:TRP:HE1	1:B:1026:GLN:NE2	2.14	0.46
1:A:62:THR:HB	1:A:121:THR:HG22	1.98	0.46
1:A:127:TYR:N	1:A:128:PRO:HD3	2.31	0.46
1:B:1402:TYR:HB3	1:B:1406:ALA:HB3	1.97	0.46
1:B:1248:THR:HB	1:B:1469:TYR:HD1	1.78	0.46
1:B:1334:GLU:HA	1:B:1338:GLN:O	2.16	0.46
1:B:1087:ASN:HD21	1:B:1142:ILE:H	1.62	0.45
1:A:239:HIS:CE1	1:A:241:GLN:OE1	2.65	0.45
1:B:1438:VAL:HG12	1:B:1450:LEU:CG	2.45	0.45
1:A:219:GLY:HA3	1:A:223:LEU:HD13	1.98	0.45
1:B:1006:ILE:CG2	1:B:1480:LEU:HD11	2.46	0.45
1:B:1103:LEU:HD22	1:B:1107:ILE:HG13	1.99	0.45
1:B:1248:THR:CG2	1:B:1293:LEU:O	2.64	0.45
1:A:103:LEU:HD22	1:A:107:ILE:HG13	2.00	0.44
1:B:1220:ASN:ND2	1:B:1246:ILE:HD11	2.32	0.44
1:B:1234:GLN:O	1:B:1236:PRO:HD3	2.17	0.44
1:B:1010:TRP:NE1	1:B:1026:GLN:HE21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1017:LEU:HD13	1:B:1033:VAL:HG21	1.99	0.44
1:B:1038:VAL:CG2	1:B:1046:VAL:CG1	2.94	0.44
1:B:1454:ILE:HG12	1:B:1454:ILE:H	1.50	0.44
1:A:241:GLN:HG3	1:A:474:VAL:HB	1.98	0.44
1:A:181:ASN:C	1:A:181:ASN:HD22	2.26	0.43
1:A:27:MET:HE2	1:A:136:PRO:HG2	2.01	0.43
1:B:1010:TRP:HE1	1:B:1026:GLN:HE21	1.66	0.43
1:B:1250:MET:HB3	1:B:1250:MET:HE2	1.75	0.43
1:A:470:ILE:HG21	1:A:470:ILE:HD13	1.18	0.43
1:B:1459:HIS:HD2	2:B:4:HOH:O	2.00	0.43
1:A:347:ILE:HG23	2:A:593:HOH:O	2.18	0.43
1:B:1146:GLN:HE21	1:B:1158:ALA:H	1.66	0.43
1:B:1226:LEU:HD22	1:B:1352:LEU:CD2	2.49	0.43
1:B:1038:VAL:HG21	1:B:1046:VAL:HG13	1.98	0.43
1:A:382:TYR:O	1:A:386:ARG:HG3	2.18	0.43
1:A:40:TYR:OH	1:A:44:GLY:HA2	2.18	0.42
1:A:94:ASN:CG	1:A:97:ARG:HG3	2.44	0.42
1:A:38:VAL:CG1	1:A:46:VAL:HG11	2.49	0.42
1:A:227:ASP:HB3	1:A:284:TYR:CE2	2.54	0.42
1:A:413:VAL:HA	1:A:414:PRO:HD3	1.85	0.42
1:A:381:ILE:HG23	1:A:393:ILE:HD11	2.02	0.42
1:A:63:TRP:CD1	1:A:63:TRP:N	2.88	0.42
1:A:320:GLU:HG2	1:A:333:ARG:HH22	1.85	0.42
1:B:1142:ILE:HG23	1:B:1147:PHE:HE2	1.85	0.42
1:B:1189:PRO:HB3	1:B:1495:GLU:HA	2.00	0.42
1:B:1434:GLU:O	1:B:1438:VAL:HG13	2.20	0.42
1:B:1278:LEU:C	1:B:1278:LEU:HD23	2.44	0.42
1:A:43:ASP:OD1	1:A:44:GLY:N	2.52	0.42
1:A:58:GLU:HB2	1:A:62:THR:CG2	2.40	0.42
1:A:373:LEU:C	1:A:374:ILE:HD13	2.45	0.41
1:A:235:ASN:C	1:A:235:ASN:OD1	2.62	0.41
1:B:1347:ILE:C	1:B:1347:ILE:HD12	2.45	0.41
1:A:220:ASN:ND2	1:A:222:GLY:N	2.48	0.41
1:B:1008:THR:HG22	1:B:1216:LEU:O	2.20	0.41
1:B:1103:LEU:HD21	1:B:1129:PHE:HD2	1.85	0.41
1:B:1038:VAL:HG21	1:B:1046:VAL:HG11	2.02	0.41
1:A:8:THR:CG2	1:A:216:LEU:O	2.66	0.41
1:B:1113:LEU:HB2	1:B:1117:GLU:HB2	2.02	0.41
1:B:1020:HIS:HE1	1:B:1140:ARG:O	2.04	0.41
1:A:18:ASN:HA	1:A:156:ILE:HD12	2.02	0.41
1:A:276:LYS:HE3	2:A:848:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:PHE:HZ	1:B:1494:PHE:CE1	2.39	0.41
1:B:1201:ASP:HA	1:B:1202:PRO:HD3	1.93	0.41
1:B:1020:HIS:HD2	1:B:1152:THR:OG1	2.04	0.41
1:B:1094:ASN:HB2	1:B:1153:MET:HG2	2.02	0.41
1:B:1157:LYS:HB3	1:B:1158:ALA:H	1.68	0.40
1:A:103:LEU:HD21	1:A:129:PHE:HD2	1.84	0.40
1:B:1036:PRO:HB2	1:B:1038:VAL:O	2.22	0.40
1:B:1191:ILE:H	1:B:1191:ILE:HG12	1.71	0.40
1:B:1012:VAL:HG22	1:B:1013:ASN:H	1.87	0.40
1:B:1438:VAL:CG1	1:B:1450:LEU:CB	2.71	0.40
1:B:1095:ARG:NH2	1:B:1107:ILE:O	2.55	0.40
1:B:1206:ALA:HB1	1:B:1228:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

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	494/502 (98%)	476 (96%)	17 (3%)	1 (0%)	43	31
1	B	494/502 (98%)	458 (93%)	28 (6%)	8 (2%)	7	2
All	All	988/1004 (98%)	934 (94%)	45 (5%)	9 (1%)	14	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1058	GLU
1	B	1056	HIS
1	B	1157	LYS
1	B	1057	SER
1	B	1221	GLU
1	B	1125	ALA

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Mol	Chain	Res	Type
1	A	157	LYS
1	B	1114	SER
1	B	1198	VAL

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	421/425 (99%)	369 (88%)	52 (12%)	4	0
1	B	421/425 (99%)	353 (84%)	68 (16%)	2	0
All	All	842/850 (99%)	722 (86%)	120 (14%)	3	0

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	8	THR
1	A	14	VAL
1	A	38	VAL
1	A	46	VAL
1	A	52	LYS
1	A	57	SER
1	A	58	GLU
1	A	59	ASP
1	A	62	THR
1	A	71	VAL
1	A	75	ASN
1	A	80	ASP
1	A	82	GLU
1	A	101	LEU
1	A	103	LEU
1	A	111	LYS
1	A	137	ARG
1	A	138	PRO
1	A	156	ILE

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	172	LEU
1	A	188	LYS
1	A	214	ILE
1	A	216	LEU
1	A	220	ASN
1	A	221	GLU
1	A	226	LEU
1	A	241	GLN
1	A	245	PRO
1	A	249	VAL
1	A	306	LYS
1	A	326	LEU
1	A	341	ARG
1	A	345	SER
1	A	347	ILE
1	A	373	LEU
1	A	377	GLU
1	A	389	ARG
1	A	415	SER
1	A	439	LEU
1	A	444	GLU
1	A	447	ARG
1	A	450	LEU
1	A	465	LEU
1	A	470	ILE
1	A	476	SER
1	A	479	GLU
1	A	480	LEU
1	A	482	ASN
1	A	483	ILE
1	A	498	LYS
1	B	1005	GLU
1	B	1007	THR
1	B	1014	VAL
1	B	1046	VAL
1	B	1052	LYS
1	B	1055	THR
1	B	1056	HIS
1	B	1059	ASP
1	B	1061	LYS
1	B	1062	THR

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Mol	Chain	Res	Type
1	B	1068	ARG
1	B	1080	ASP
1	B	1095	ARG
1	B	1101	LEU
1	B	1103	LEU
1	B	1110	VAL
1	B	1111	LYS
1	B	1115	LYS
1	B	1120	ILE
1	B	1127	TYR
1	B	1137	ARG
1	B	1148	LYS
1	B	1149	ASN
1	B	1151	GLU
1	B	1154	ASN
1	B	1156	ILE
1	B	1157	LYS
1	B	1167	LEU
1	B	1177	VAL
1	B	1188	LYS
1	B	1191	ILE
1	B	1204	THR
1	B	1207	VAL
1	B	1213	ASP
1	B	1216	LEU
1	B	1221	GLU
1	B	1226	LEU
1	B	1235	ASN
1	B	1241	GLN
1	B	1244	GLN
1	B	1246	ILE
1	B	1247	GLU
1	B	1248	THR
1	B	1253	LEU
1	B	1276	LYS
1	B	1319	LEU
1	B	1330	LYS
1	B	1344	LEU
1	B	1347	ILE
1	B	1367	ILE
1	B	1371	VAL
1	B	1373	LEU

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Mol	Chain	Res	Type
1	B	1374	ILE
1	B	1386	ARG
1	B	1389	ARG
1	B	1395	HIS
1	B	1427	ASP
1	B	1439	LEU
1	B	1450	LEU
1	B	1454	ILE
1	B	1465	LEU
1	B	1476	SER
1	B	1477	LYS
1	B	1479	GLU
1	B	1483	ILE
1	B	1495	GLU
1	B	1496	GLN
1	B	1498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	20	HIS
1	A	26	GLN
1	A	75	ASN
1	A	87	ASN
1	A	94	ASN
1	A	106	GLN
1	A	131	GLN
1	A	146	GLN
1	A	174	GLN
1	A	181	ASN
1	A	197	ASN
1	A	220	ASN
1	A	239	HIS
1	A	446	GLN
1	A	448	GLN
1	A	459	HIS
1	A	496	GLN
1	B	1013	ASN
1	B	1020	HIS
1	B	1026	GLN
1	B	1087	ASN

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Mol	Chain	Res	Type
1	B	1094	ASN
1	B	1106	GLN
1	B	1174	GLN
1	B	1181	ASN
1	B	1220	ASN
1	B	1281	ASN
1	B	1309	GLN
1	B	1385	GLN
1	B	1395	HIS
1	B	1420	GLN
1	B	1446	GLN
1	B	1459	HIS

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	496/502 (98%)	-0.18	10 (2%) 65 68	10, 22, 42, 67	0
1	B	496/502 (98%)	0.75	106 (21%) 2 2	9, 40, 81, 94	0
All	All	992/1004 (98%)	0.29	116 (11%) 9 8	9, 26, 72, 94	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1073	PHE	4.7
1	B	1071	VAL	4.5
1	B	1079	PHE	4.4
1	B	1172	LEU	4.1
1	B	1185	TRP	3.9
1	B	1142	ILE	3.9
1	B	1175	TYR	3.8
1	B	1199	ILE	3.7
1	B	1189	PRO	3.7
1	B	1165	TRP	3.7
1	B	1067	LEU	3.6
1	B	1198	VAL	3.6
1	B	1159	PRO	3.5
1	B	1143	ALA	3.5
1	B	1033	VAL	3.5
1	B	1158	ALA	3.5
1	B	1078	PRO	3.4
1	B	1081	ALA	3.4
1	B	1145	SER	3.4
1	B	1177	VAL	3.3
1	B	1155	GLY	3.2
1	B	1153	MET	3.2
1	B	1146	GLN	3.2
1	B	1497	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1147	PHE	3.2
1	B	1074	SER	3.1
1	B	1099	ALA	3.1
1	B	1150	HIS	3.1
1	B	1014	VAL	3.1
1	B	1179	VAL	3.1
1	B	1160	ILE	3.0
1	B	1076	GLY	3.0
1	B	1113	LEU	3.0
1	B	1156	ILE	3.0
1	B	1178	PHE	3.0
1	B	1110	VAL	2.9
1	B	1084	ALA	2.9
1	B	1152	THR	2.9
1	A	60	GLY	2.9
1	B	1021	LEU	2.9
1	B	1163	GLY	2.8
1	B	1116	THR	2.8
1	B	1207	VAL	2.8
1	A	125	ALA	2.8
1	B	1195	THR	2.8
1	B	1162	THR	2.7
1	B	1235	ASN	2.7
1	A	442	HIS	2.7
1	A	63	TRP	2.7
1	B	1090	ALA	2.7
1	B	1019	PRO	2.7
1	B	1191	ILE	2.7
1	B	1012	VAL	2.6
1	B	1056	HIS	2.6
1	B	1157	LYS	2.6
1	B	1050	LEU	2.6
1	B	1112	ALA	2.6
1	B	1075	ASN	2.5
1	B	1023	THR	2.5
1	B	1024	PRO	2.5
1	B	1149	ASN	2.5
1	A	57	SER	2.5
1	B	1214	ILE	2.5
1	B	1063	TRP	2.5
1	B	1476	SER	2.4
1	B	1442	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	415	SER	2.4
1	B	1066	THR	2.4
1	B	1091	VAL	2.4
1	B	1148	LYS	2.4
1	B	1151	GLU	2.4
1	B	1080	ASP	2.3
1	B	1092	LEU	2.3
1	B	1055	THR	2.3
1	B	1059	ASP	2.3
1	B	1100	TRP	2.3
1	B	1211	THR	2.3
1	B	1184	TYR	2.3
1	B	1083	ALA	2.3
1	B	1499	PRO	2.3
1	B	1070	ASP	2.3
1	B	1220	ASN	2.3
1	B	1118	LEU	2.3
1	B	1144	PRO	2.2
1	B	1045	SER	2.2
1	A	56	HIS	2.2
1	A	58	GLU	2.2
1	B	1236	PRO	2.2
1	B	1382	TYR	2.2
1	B	1072	LYS	2.2
1	B	1167	LEU	2.2
1	A	128	PRO	2.2
1	B	1190	ALA	2.2
1	B	1006	ILE	2.2
1	B	1194	ILE	2.2
1	B	1038	VAL	2.2
1	B	1481	GLY	2.2
1	B	1237	ALA	2.2
1	B	1096	GLN	2.1
1	B	1057	SER	2.1
1	B	1212	GLY	2.1
1	B	1088	PHE	2.1
1	A	382	TYR	2.1
1	B	1047	ILE	2.1
1	B	1161	GLY	2.1
1	B	1187	GLU	2.1
1	B	1085	ALA	2.1
1	B	1069	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1215	ASP	2.1
1	B	1017	LEU	2.1
1	B	1064	THR	2.0
1	B	1181	ASN	2.0
1	B	1046	VAL	2.0
1	B	1166	ILE	2.0
1	B	1044	GLY	2.0
1	B	1238	TYR	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.