Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2021 – 09:14 PM EDT

PDB ID	:	1UIU
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

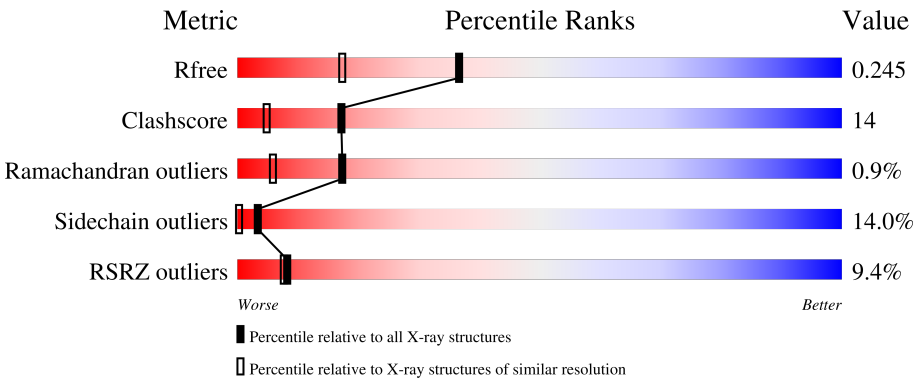
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 <=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% 5% ••
1	B	502	17% 64% 27% 7% ••

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	496	3941	2525	667	739	10	0	0	0
1	B	496	3941	2525	667	739	10	0	0	0

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.

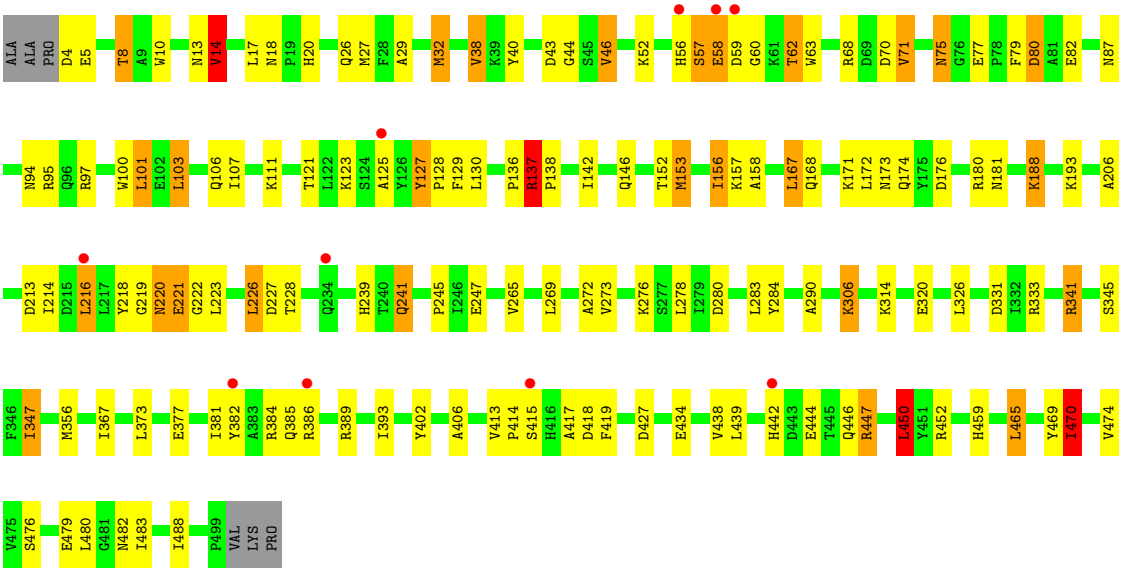
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	350	350	350	0	0
2	B	195	195	195	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

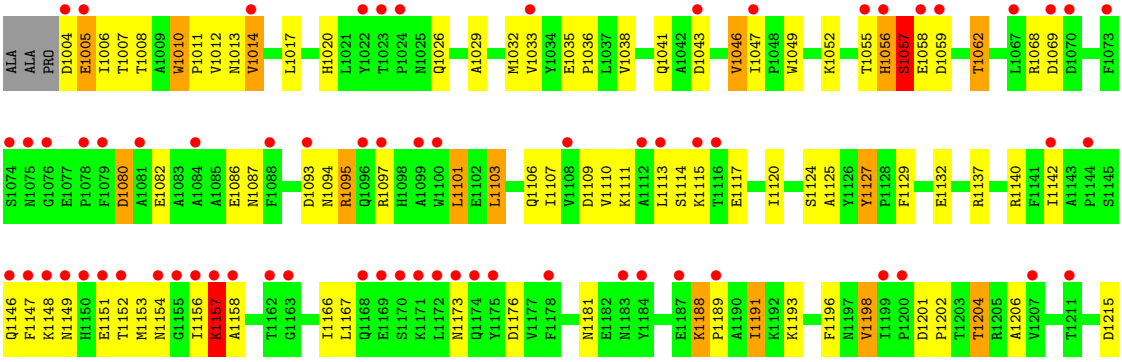
• Molecule 1: Nickel-binding periplasmic protein

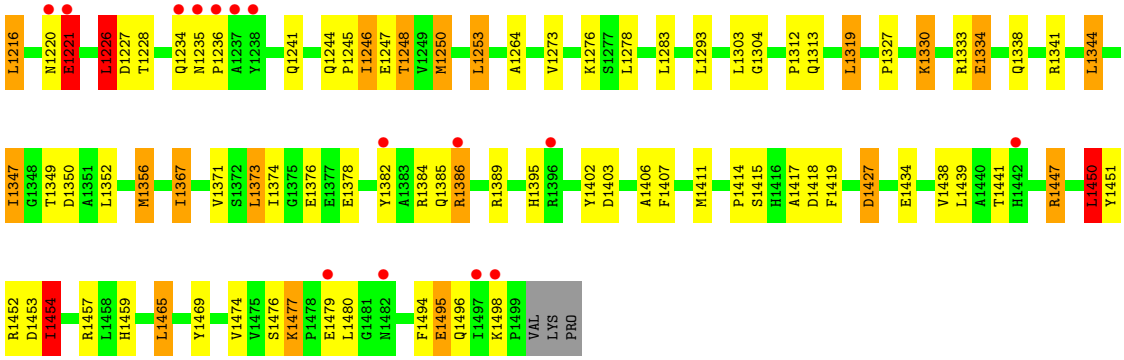
Chain A:



• Molecule 1: Nickel-binding periplasmic protein

Chain B:




L1216
N1220
E1221
L1226
D1227
T1228
Q1234
N1235
P1236
A1237
Y1238
Q1241
Q1244
P1245
I1246
E1247
T1248
V1249
M1250
L1253
A1264
V1273
K1276
S1277
L1278
L1283
L1293
L1303
G1304
P1312
Q1313
L1319
P1327
K1330
R1333
E1334
Q1338
R1341
L1344
I1347
G1348
T1349
D1350
A1351
L1352
M1356
I1367
V1371
S1372
L1373
I1374
G1375
E1376
E1377
E1378
Y1382
A1383
R1384
Q1385
R1386
R1389
H1395
R1396
Y1402
D1403
A1406
F1407
M1411
P1414
S1415
H1416
A1417
D1418
F1419
D1427
E1434
V1438
L1439
A1440
T1441
H1442
R1447
L1450
Y1451
R1452
D1453
I1454
R1457
L1458
H1459
L1465
Y1469
V1474
V1475
S1476
K1477
P1478
E1479
L1480
G1481
N1482
F1494
E1495
Q1496
I1497
K1498
P1499
VAL
LYS
PRO

4 Data and refinement statistics (i)

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) 87.8 (19.96-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.34 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	1.01	3/4044 (0.1%)	1.10	21/5508 (0.4%)
1	B	0.90	6/4044 (0.1%)	1.09	31/5508 (0.6%)
All	All	0.96	9/8088 (0.1%)	1.09	52/11016 (0.5%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1427	ASP	CB-CG	-9.15	1.32	1.51
1	A	32	MET	SD-CE	-6.65	1.40	1.77
1	B	1334	GLU	CD-OE1	5.90	1.32	1.25
1	B	1333	ARG	CG-CD	5.88	1.66	1.51
1	B	1356	MET	SD-CE	-5.69	1.46	1.77
1	A	356	MET	SD-CE	-5.62	1.46	1.77
1	B	1427	ASP	CA-CB	5.61	1.66	1.53
1	A	273	VAL	CB-CG1	5.56	1.64	1.52
1	B	1264	ALA	CA-CB	5.37	1.63	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1427	ASP	CB-CG-OD1	-20.86	99.53	118.30
1	B	1427	ASP	CB-CG-OD2	19.62	135.96	118.30
1	B	1303	LEU	C-N-CA	-12.50	96.06	122.30
1	A	470	ILE	CG1-CB-CG2	-11.02	87.16	111.40
1	A	137	ARG	NE-CZ-NH1	10.64	125.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	B	1341	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	14	VAL	CG1-CB-CG2	8.48	124.47	110.90
1	A	153	MET	CG-SD-CE	-8.06	87.31	100.20
1	B	1447	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	447	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	465	LEU	CB-CG-CD2	7.75	124.18	111.00
1	A	70	ASP	CB-CG-OD2	6.83	124.44	118.30
1	B	1253	LEU	CB-CG-CD2	6.82	122.58	111.00
1	A	213	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	427	ASP	CB-CG-OD2	6.62	124.25	118.30
1	B	1253	LEU	CB-CG-CD1	6.56	122.16	111.00
1	B	1465	LEU	CB-CG-CD1	6.45	121.97	111.00
1	A	280	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	1004	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	452	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	80	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	1344	LEU	CB-CG-CD2	6.23	121.59	111.00
1	B	1341	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	B	1080	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	418	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	1450	LEU	CB-CG-CD1	6.11	121.39	111.00
1	B	1453	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	167	LEU	CB-CG-CD2	5.79	120.84	111.00
1	B	1447	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	1303	LEU	O-C-N	-5.64	113.61	123.20
1	B	1043	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	1227	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	1093	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	331	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	1457	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	1454	ILE	CG1-CB-CG2	-5.32	99.69	111.40
1	B	1109	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	1371	VAL	CG1-CB-CG2	5.31	119.39	110.90
1	B	1226	LEU	CB-CG-CD2	5.23	119.89	111.00
1	B	1176	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	1250	MET	CG-SD-CE	-5.21	91.87	100.20
1	B	1350	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	1319	LEU	CB-CG-CD1	5.19	119.82	111.00
1	B	1427	ASP	N-CA-CB	-5.15	101.33	110.60
1	A	176	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	341	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1373	LEU	CB-CG-CD1	5.07	119.62	111.00
1	A	137	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	450	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	14	VAL	N-CA-CB	-5.00	100.49	111.50
1	B	1403	ASP	CB-CG-OD2	5.00	122.80	118.30

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 (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	3941	0	3891	106	0
1	B	3941	0	3891	111	0
2	A	350	0	0	13	0
2	B	195	0	0	3	0
All	All	8427	0	7782	217	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 (217) 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	1.01
1:A:106:GLN:HE21	1:A:123:LYS:HB2	1.25	0.99
1:B:1082:GLU:O	1:B:1086:GLU:HG2	1.64	0.97
1:A:220:ASN:ND2	1:A:222:GLY:H	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1029:ALA:HA	1:B:1032:MET:HE2	1.60	0.81
1:B:1220:ASN:HB3	1:B:1221:GLU:HG3	1.63	0.81
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: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:A:153:MET:CE	2:A:660:HOH:O	2.39	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:A:438:VAL:HG12	1:A:450:LEU:HG	1.77	0.67
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:1441:THR:HG23	1:B:1447:ARG:HD3	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1313:GLN:CD	1:B:1313:GLN:H	2.03	0.62
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:220:ASN:HD22	1:A:220:ASN:C	2.03	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:A:27:MET:HE1	2:A:590:HOH:O	2.01	0.60
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: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:1029:ALA:HA	1:B:1032:MET:CE	2.30	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1312:PRO:CA	1:B:1367:ILE:HD11	2.33	0.56
1:B:1407:PHE:CE1	1:B:1411:MET:HE3	2.40	0.55
1:B:1385:GLN:HB3	1:B:1417:ALA:HB2	1.88	0.55
1:B:1407:PHE:CE1	1:B:1411:MET:HE2	2.41	0.55
1:A:153:MET:HE3	2:A:660:HOH:O	2.06	0.54
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: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:1014:VAL:HG13	1:B:1017:LEU:HD21	1.91	0.53
1:A:278:LEU:C	1:A:278:LEU:HD23	2.29	0.52
1:B:1278:LEU:HD21	1:B:1356:MET:HE3	1.90	0.52
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: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:B:1014:VAL:HG22	1:B:1029:ALA:HB2	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1278:LEU:HD21	1:B:1356:MET:CE	2.43	0.49
1:B:1035:GLU:CD	1:B:1049:TRP:HE1	2.17	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:A:153:MET:HE1	2:A:660:HOH:O	2.06	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: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: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:A:220:ASN:ND2	1:A:220:ASN:C	2.69	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:171:LYS:HD3	1:A:174:GLN:CD	2.37	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:HG3	1:A:474:VAL:HB	1.98	0.44
1:B:1283:LEU:HD11	1:B:1356:MET:HE3	1.98	0.44
1:B:1010:TRP:HE1	1:B:1026:GLN:HE21	1.66	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:A:27:MET:CE	2:A:590:HOH:O	2.61	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:479:GLU:CD	1:A:479:GLU:H	2.22	0.43
1:A:40:TYR:OH	1:A:44:GLY:HA2	2.18	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: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:B:1407:PHE:CD1	1:B:1411:MET:HE3	2.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	494/502 (98%)	476 (96%)	17 (3%)	1 (0%)	47 33
1	B	494/502 (98%)	458 (93%)	28 (6%)	8 (2%)	9 2
All	All	988/1004 (98%)	934 (94%)	45 (5%)	9 (1%)	17 6

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
1	A	157	LYS
1	B	1114	SER
1	B	1198	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	421/425 (99%)	368 (87%)	53 (13%)	4 0
1	B	421/425 (99%)	356 (85%)	65 (15%)	2 0
All	All	842/850 (99%)	724 (86%)	118 (14%)	3 0

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	8	THR
1	A	14	VAL
1	A	38	VAL
1	A	46	VAL
1	A	52	LYS
1	A	56	HIS
1	A	57	SER
1	A	58	GLU
1	A	59	ASP
1	A	62	THR
1	A	68	ARG
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	127	TYR
1	A	137	ARG
1	A	138	PRO
1	A	156	ILE
1	A	167	LEU
1	A	172	LEU
1	A	181	ASN
1	A	188	LYS

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Mol	Chain	Res	Type
1	A	214	ILE
1	A	216	LEU
1	A	218	TYR
1	A	220	ASN
1	A	221	GLU
1	A	226	LEU
1	A	241	GLN
1	A	245	PRO
1	A	306	LYS
1	A	326	LEU
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	480	LEU
1	A	482	ASN
1	A	483	ILE
1	B	1005	GLU
1	B	1007	THR
1	B	1010	TRP
1	B	1014	VAL
1	B	1046	VAL
1	B	1052	LYS
1	B	1055	THR
1	B	1056	HIS
1	B	1057	SER
1	B	1059	ASP
1	B	1062	THR
1	B	1068	ARG
1	B	1069	ASP
1	B	1080	ASP
1	B	1095	ARG
1	B	1097	ARG

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Mol	Chain	Res	Type
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	1188	LYS
1	B	1191	ILE
1	B	1204	THR
1	B	1216	LEU
1	B	1221	GLU
1	B	1226	LEU
1	B	1235	ASN
1	B	1244	GLN
1	B	1246	ILE
1	B	1247	GLU
1	B	1248	THR
1	B	1250	MET
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	1373	LEU
1	B	1374	ILE
1	B	1386	ARG
1	B	1389	ARG
1	B	1427	ASP
1	B	1439	LEU
1	B	1450	LEU
1	B	1454	ILE

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Mol	Chain	Res	Type
1	B	1465	LEU
1	B	1476	SER
1	B	1477	LYS
1	B	1479	GLU
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 (36) 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	146	GLN
1	A	168	GLN
1	A	174	GLN
1	A	181	ASN
1	A	197	ASN
1	A	220	ASN
1	A	239	HIS
1	A	416	HIS
1	A	420	GLN
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	1075	ASN
1	B	1087	ASN
1	B	1094	ASN
1	B	1106	GLN
1	B	1146	GLN
1	B	1181	ASN
1	B	1220	ASN
1	B	1309	GLN
1	B	1385	GLN

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Mol	Chain	Res	Type
1	B	1395	HIS
1	B	1420	GLN
1	B	1446	GLN
1	B	1448	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 monosaccharides 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	496/502 (98%)	-0.23	10 (2%)	65	64	10, 22, 42, 67	0
1	B	496/502 (98%)	0.60	83 (16%)	1	1	9, 40, 81, 94	0
All	All	992/1004 (98%)	0.19	93 (9%)	8	8	9, 26, 72, 94	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1067	LEU	6.1
1	B	1149	ASN	5.2
1	B	1158	ALA	5.0
1	B	1148	LYS	4.6
1	B	1207	VAL	4.4
1	B	1175	TYR	4.4
1	B	1024	PRO	4.3
1	B	1078	PRO	4.3
1	B	1075	ASN	4.1
1	B	1168	GLN	4.1
1	B	1382	TYR	4.1
1	B	1113	LEU	4.0
1	B	1211	THR	4.0
1	B	1079	PHE	4.0
1	B	1069	ASP	3.9
1	B	1386	ARG	3.9
1	B	1116	THR	3.8
1	B	1497	ILE	3.7
1	B	1023	THR	3.7
1	B	1154	ASN	3.7
1	B	1146	GLN	3.6
1	B	1058	GLU	3.6
1	B	1070	ASP	3.5
1	B	1174	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1172	LEU	3.4
1	B	1147	PHE	3.3
1	B	1056	HIS	3.3
1	A	58	GLU	3.3
1	B	1096	GLN	3.3
1	B	1183	ASN	3.3
1	B	1097	ARG	3.2
1	B	1043	ASP	3.2
1	B	1479	GLU	3.2
1	B	1235	ASN	3.2
1	B	1200	PRO	3.2
1	B	1108	VAL	3.1
1	B	1234	GLN	3.1
1	A	382	TYR	3.0
1	A	415	SER	3.0
1	B	1099	ALA	3.0
1	B	1022	TYR	2.9
1	A	59	ASP	2.9
1	B	1221	GLU	2.9
1	B	1084	ALA	2.9
1	B	1498	LYS	2.9
1	B	1074	SER	2.8
1	B	1156	ILE	2.8
1	B	1047	ILE	2.8
1	B	1073	PHE	2.8
1	B	1482	ASN	2.8
1	B	1163	GLY	2.7
1	B	1189	PRO	2.7
1	B	1076	GLY	2.7
1	B	1142	ILE	2.6
1	B	1100	TRP	2.6
1	B	1155	GLY	2.6
1	B	1178	PHE	2.6
1	B	1199	ILE	2.5
1	B	1150	HIS	2.5
1	B	1236	PRO	2.5
1	B	1144	PRO	2.5
1	A	125	ALA	2.4
1	A	56	HIS	2.4
1	B	1173	ASN	2.4
1	B	1171	LYS	2.4
1	B	1151	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1152	THR	2.3
1	B	1088	PHE	2.3
1	B	1093	ASP	2.3
1	B	1220	ASN	2.3
1	B	1059	ASP	2.3
1	B	1014	VAL	2.2
1	B	1081	ALA	2.2
1	B	1442	HIS	2.2
1	B	1238	TYR	2.2
1	B	1033	VAL	2.2
1	B	1157	LYS	2.2
1	B	1237	ALA	2.2
1	B	1055	THR	2.2
1	B	1396	ARG	2.2
1	B	1115	LYS	2.2
1	A	216	LEU	2.1
1	B	1184	TYR	2.1
1	B	1162	THR	2.1
1	B	1169	GLU	2.1
1	A	234	GLN	2.1
1	B	1005	GLU	2.1
1	B	1187	GLU	2.1
1	B	1170	SER	2.1
1	B	1004	ASP	2.0
1	A	442	HIS	2.0
1	B	1112	ALA	2.0
1	A	386	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.