



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:38 PM GMT

PDB ID : 1UIV  
Title : Crystal structures of the liganded and unliganded nickel binding protein NikA from Escherichia coli (Nickel liganded form)  
Authors : Heddle, J.; Scott, D.J.; Unzai, S.; Park, S.-Y.; Tame, J.R.H.  
Deposited on : 2003-07-22  
Resolution : 1.95 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.

---

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

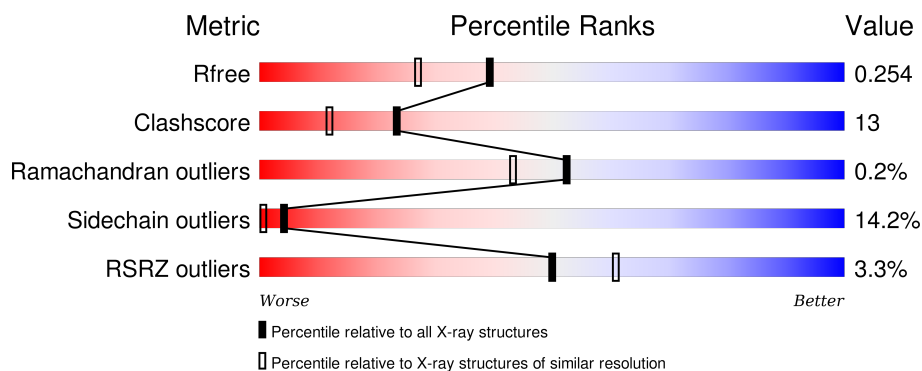
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	502	<div> <div>4%</div> <div>71%</div> <div>21%</div> <div>7%</div> <div>..</div> </div>
1	B	502	<div> <div>3%</div> <div>67%</div> <div>23%</div> <div>7%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8382 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	497	Total	C	N	O	S	0	0	0
			3948	2530	668	740	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	UNP P33590
B	1361	ARG	GLN	ENGINEERED	UNP P33590

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		

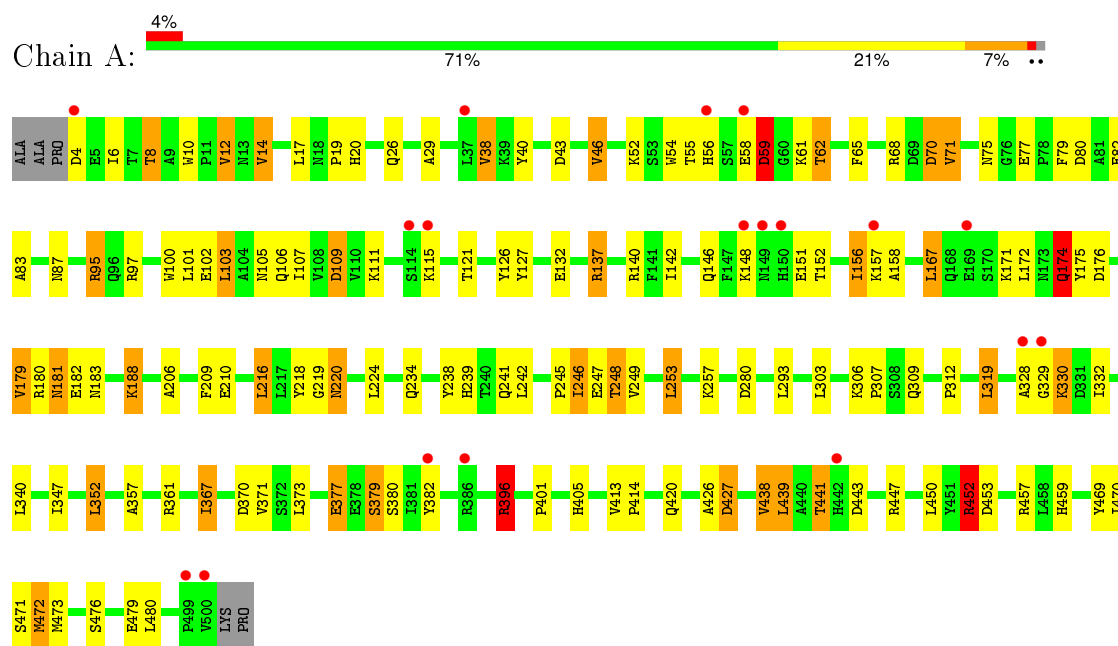
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total	O	0	0
			258	258		
3	B	233	Total	O	0	0
			233	233		

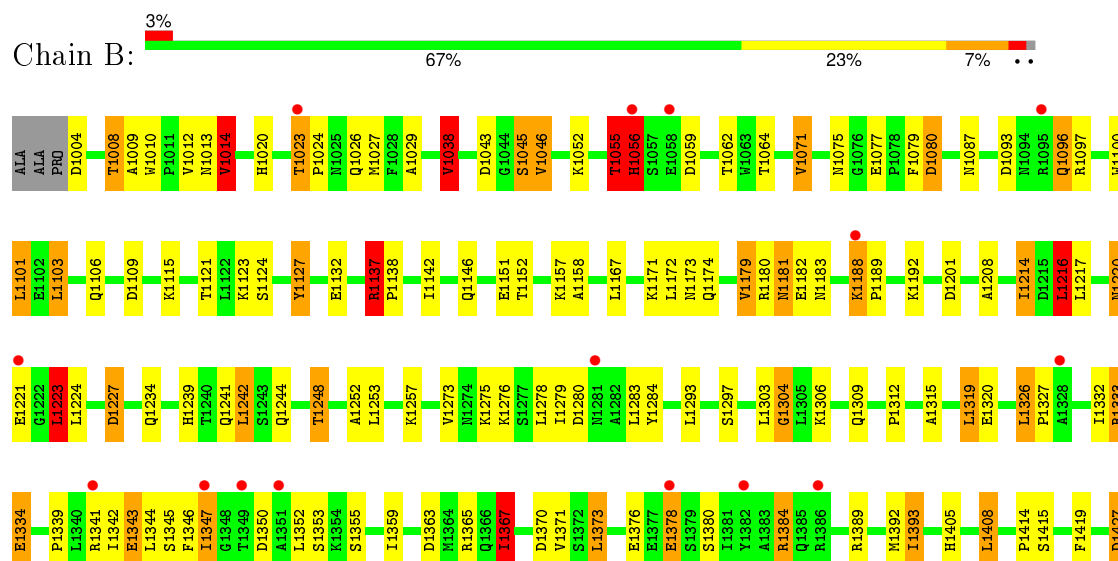
### 3 Residue-property plots

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: Nickel-binding periplasmic protein



#### • Molecule 1: Nickel-binding periplasmic protein



L1439	A1440	T1441	H1442	D1443	E1444	T1445	Q1446	R1447
L1450	I1454	H1459	D1460	E1461	L1465	Y1469	I1470	S1471
M1472	V1475	S1476	E1479	N1482	Y1485	K1498	P1499	VAL
LYS	PRO							

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.72Å 192.81Å 75.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.95) 93.7 (19.90-1.94)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.27 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.199 , 0.254 0.201 , 0.254	Depositor DCC
$R_{free}$ test set	3588 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 70727 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.99	5/4051 (0.1%)	1.21	36/5518 (0.7%)
1	B	1.00	1/4044 (0.0%)	1.14	38/5508 (0.7%)
All	All	0.99	6/8095 (0.1%)	1.17	74/11026 (0.7%)

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	1	1
1	B	0	2
All	All	1	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1444	GLU	CD-OE1	9.53	1.36	1.25
1	A	479	GLU	CD-OE2	7.66	1.34	1.25
1	A	174	GLN	CB-CG	7.65	1.73	1.52
1	A	452	ARG	NE-CZ	-5.93	1.25	1.33
1	A	452	ARG	CG-CD	5.68	1.66	1.51
1	A	396	ARG	CB-CG	-5.25	1.38	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	NE-CZ-NH2	-24.79	107.90	120.30
1	A	4	ASP	CB-CA-C	19.10	148.59	110.40
1	A	452	ARG	NE-CZ-NH1	15.58	128.09	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1303	LEU	C-N-CA	-12.21	96.66	122.30
1	B	1447	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	B	1447	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	A	427	ASP	CB-CG-OD2	9.98	127.28	118.30
1	A	352	LEU	CA-CB-CG	9.85	137.96	115.30
1	B	1201	ASP	CB-CG-OD2	9.35	126.72	118.30
1	A	43	ASP	CB-CG-OD2	8.75	126.17	118.30
1	B	1333	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	1333	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	B	1367	ILE	CG1-CB-CG2	8.28	129.62	111.40
1	A	137	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	137	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	1080	ASP	CB-CG-OD2	8.16	125.64	118.30
1	B	1137	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	1280	ASP	CB-CG-OD2	7.59	125.14	118.30
1	B	1216	LEU	CA-CB-CG	7.47	132.48	115.30
1	A	12	VAL	CG1-CB-CG2	7.44	122.80	110.90
1	A	70	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	1350	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	452	ARG	CG-CD-NE	-7.28	96.51	111.80
1	A	329	GLY	N-CA-C	-7.10	95.36	113.10
1	B	1427	ASP	CB-CG-OD2	7.02	124.62	118.30
1	B	1004	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	438	VAL	CB-CA-C	-6.92	98.25	111.40
1	B	1443	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	457	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	396	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	1109	ASP	CB-CG-OD2	6.74	124.36	118.30
1	B	1038	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	A	427	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	A	414	PRO	C-N-CA	-6.38	105.74	121.70
1	A	452	ARG	CD-NE-CZ	6.37	132.52	123.60
1	B	1056	HIS	N-CA-CB	-6.31	99.24	110.60
1	A	453	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	1223	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	438	VAL	CG1-CB-CG2	5.99	120.49	110.90
1	A	396	ARG	CG-CD-NE	5.97	124.34	111.80
1	A	340	LEU	CB-CG-CD2	-5.97	100.86	111.00
1	B	1179	VAL	CG1-CB-CG2	5.92	120.38	110.90
1	B	1045	SER	CB-CA-C	-5.88	98.94	110.10
1	B	1242	LEU	CB-CG-CD2	5.84	120.93	111.00
1	B	1012	VAL	CG1-CB-CG2	5.82	120.21	110.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	VAL	CG1-CB-CG2	5.78	120.16	110.90
1	A	176	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	1326	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	12	VAL	N-CA-CB	-5.60	99.17	111.50
1	A	109	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	1103	LEU	CB-CG-CD2	5.55	120.44	111.00
1	B	1465	LEU	CB-CG-CD1	5.55	120.43	111.00
1	B	1014	VAL	CG1-CB-CG2	5.49	119.69	110.90
1	B	1059	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	59	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	1408	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	1470	ILE	CB-CA-C	-5.29	101.03	111.60
1	A	253	LEU	CB-CG-CD1	5.28	119.97	111.00
1	B	1303	LEU	O-C-N	-5.26	114.26	123.20
1	A	443	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	140	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	1476	SER	CA-CB-OG	-5.18	97.21	111.20
1	A	280	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	1137	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	396	ARG	CB-CA-C	5.10	120.61	110.40
1	B	1319	LEU	CB-CG-CD1	5.10	119.67	111.00
1	B	1080	ASP	CB-CA-C	-5.09	100.21	110.40
1	A	167	LEU	CB-CG-CD2	5.05	119.59	111.00
1	B	1227	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	426	ALA	C-N-CA	5.03	134.26	121.70
1	B	1363	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	1303	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	A	439	LEU	CB-CG-CD1	5.02	119.53	111.00
1	A	319	LEU	CB-CG-CD1	5.00	119.51	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	ASP	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ALA	Peptide
1	B	1055	THR	Peptide
1	B	1304	GLY	Peptide

## 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	3948	0	3900	105	0
1	B	3941	0	3891	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	258	0	0	4	0
3	B	233	0	0	16	0
All	All	8382	0	7791	208	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 13.

All (208) 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:1315:ALA:HB3	1:B:1367:ILE:CD1	1.61	1.26
1:A:330:LYS:HB3	1:A:330:LYS:NZ	1.55	1.11
1:A:472:MET:HE3	1:A:472:MET:HA	1.32	1.08
1:A:330:LYS:HB3	1:A:330:LYS:HZ3	1.07	1.06
1:A:234:GLN:HG2	1:B:1304:GLY:HA3	1.42	0.98
1:A:472:MET:HE2	1:A:473:MET:H	1.25	0.96
1:B:1013:ASN:HD21	1:B:1173:ASN:H	1.10	0.96
1:B:1315:ALA:CB	1:B:1367:ILE:CD1	2.43	0.95
1:B:1096:GLN:CD	1:B:1096:GLN:H	1.68	0.94
1:A:377:GLU:OE1	1:A:379:SER:HB3	1.68	0.94
1:A:472:MET:CE	1:A:473:MET:H	1.83	0.91
1:B:1315:ALA:HB3	1:B:1367:ILE:HD11	1.52	0.90
1:A:248:THR:HG21	1:A:293:LEU:O	1.72	0.89
1:A:330:LYS:CB	1:A:330:LYS:NZ	2.36	0.89
1:B:1146:GLN:HE21	1:B:1158:ALA:H	1.20	0.89
1:B:1224:LEU:HB2	3:B:442:HOH:O	1.77	0.82
1:B:1315:ALA:HB3	1:B:1367:ILE:HD12	1.61	0.81
1:B:1315:ALA:HB3	1:B:1367:ILE:HD13	1.61	0.81
1:A:472:MET:CA	1:A:472:MET:HE3	2.11	0.79
1:A:38:VAL:HG13	1:A:46:VAL:CG2	2.12	0.78
1:A:377:GLU:OE1	1:A:379:SER:CB	2.32	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1220:ASN:ND2	1:B:1221:GLU:HG2	2.00	0.77
1:B:1014:VAL:HG22	1:B:1029:ALA:HB2	1.65	0.76
1:A:8:THR:HG23	1:A:216:LEU:O	1.87	0.75
1:A:361:ARG:HD3	1:A:373:LEU:CD2	2.16	0.74
1:B:1315:ALA:CB	1:B:1367:ILE:HD12	2.13	0.74
1:A:219:GLY:C	1:A:472:MET:HE1	2.06	0.74
1:B:1220:ASN:HD22	1:B:1220:ASN:C	1.91	0.74
1:B:1252:ALA:HB3	1:B:1393:ILE:HG22	1.68	0.73
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.35	0.73
1:B:1043:ASP:OD2	1:B:1045:SER:HB2	1.87	0.73
1:B:1013:ASN:HD21	1:B:1173:ASN:N	1.86	0.73
1:A:62:THR:HB	1:A:121:THR:HG22	1.71	0.73
1:A:20:HIS:HD2	1:A:152:THR:OG1	1.70	0.72
1:B:1339:PRO:HB2	1:B:1341:ARG:HG3	1.69	0.72
1:B:1341:ARG:HG2	1:B:1370:ASP:HB3	1.70	0.72
1:B:1326:LEU:HD12	3:B:170:HOH:O	1.89	0.72
1:B:1224:LEU:CB	3:B:442:HOH:O	2.33	0.71
1:B:1332:ILE:HG12	1:B:1370:ASP:HB2	1.72	0.71
1:B:1248:THR:HG21	1:B:1293:LEU:O	1.90	0.71
1:B:1013:ASN:ND2	1:B:1173:ASN:H	1.86	0.70
1:B:1239:HIS:HE1	1:B:1241:GLN:OE1	1.75	0.70
1:B:1096:GLN:CD	1:B:1096:GLN:N	2.46	0.69
1:B:1327:PRO:HG3	1:B:1334:GLU:HG2	1.74	0.69
1:A:105:ASN:HB3	3:A:740:HOH:O	1.91	0.69
1:A:68:ARG:HG2	1:A:70:ASP:OD1	1.91	0.69
1:B:1341:ARG:HD3	1:B:1370:ASP:OD2	1.93	0.69
3:A:525:HOH:O	1:B:1239:HIS:HD2	1.75	0.69
1:B:1038:VAL:HG13	1:B:1046:VAL:CG2	2.22	0.69
1:A:38:VAL:HG13	1:A:46:VAL:HG22	1.74	0.68
1:B:1052:LYS:HE3	3:B:439:HOH:O	1.92	0.68
1:A:38:VAL:HG13	1:A:46:VAL:HG21	1.76	0.68
1:A:146:GLN:HE21	1:A:158:ALA:H	1.42	0.68
1:B:1010:TRP:HE1	1:B:1026:GLN:HE21	1.43	0.67
1:A:71:VAL:HG22	1:A:79:PHE:HB3	1.77	0.67
1:B:1023:THR:HG23	3:B:399:HOH:O	1.95	0.66
1:A:103:LEU:O	1:A:103:LEU:HD23	1.95	0.65
1:A:472:MET:CE	1:A:473:MET:N	2.60	0.64
1:B:1312:PRO:HA	1:B:1367:ILE:HD11	1.78	0.64
1:B:1020:HIS:HD2	1:B:1152:THR:OG1	1.81	0.64
1:A:248:THR:CG2	1:A:293:LEU:O	2.47	0.63
1:A:132:GLU:OE1	1:A:405:HIS:NE2	2.28	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1220:ASN:ND2	1:B:1220:ASN:C	2.52	0.61
1:A:248:THR:HG22	3:A:510:HOH:O	1.99	0.61
1:B:1220:ASN:HD21	1:B:1221:GLU:HG2	1.66	0.61
1:A:10:TRP:HE1	1:A:26:GLN:NE2	1.99	0.61
1:A:68:ARG:CG	1:A:70:ASP:OD1	2.48	0.60
1:B:1071:VAL:HG22	1:B:1079:PHE:HB3	1.83	0.60
1:B:1127:TYR:CE2	1:B:1447:ARG:HD2	2.36	0.60
1:B:1347:ILE:HA	1:B:1376:GLU:O	2.01	0.60
1:B:1014:VAL:HG22	1:B:1029:ALA:CB	2.32	0.60
1:B:1279:ILE:HG12	1:B:1283:LEU:HD12	1.84	0.60
1:A:330:LYS:HB3	1:A:330:LYS:HZ2	1.64	0.59
1:A:8:THR:CG2	1:A:216:LEU:O	2.50	0.59
1:A:330:LYS:CB	1:A:330:LYS:HZ2	2.14	0.59
1:B:1217:LEU:HB2	1:B:1475:VAL:HG22	1.84	0.59
1:A:216:LEU:HD21	1:A:218:TYR:HB2	1.85	0.59
1:A:100:TRP:HA	1:A:413:VAL:HG21	1.86	0.58
1:A:239:HIS:HE1	1:A:241:GLN:OE1	1.87	0.57
1:B:1306:LYS:O	1:B:1459:HIS:HE1	1.86	0.57
1:B:1038:VAL:HG13	1:B:1046:VAL:HG22	1.85	0.57
1:B:1023:THR:CG2	3:B:399:HOH:O	2.51	0.57
1:A:248:THR:HB	1:A:469:TYR:CD1	2.40	0.57
1:A:246:ILE:HD12	1:A:470:ILE:O	2.05	0.57
1:A:377:GLU:CD	1:A:379:SER:H	2.08	0.57
1:B:1320:GLU:OE2	1:B:1333:ARG:NH2	2.38	0.56
1:A:220:ASN:N	1:A:472:MET:HE1	2.18	0.56
1:B:1009:ALA:HB2	1:B:1214:ILE:CD1	2.36	0.56
1:B:1384:ARG:HG2	1:B:1389:ARG:O	2.06	0.56
1:A:246:ILE:CD1	1:A:470:ILE:O	2.52	0.56
1:B:1132:GLU:OE1	1:B:1405:HIS:NE2	2.33	0.56
1:B:1075:ASN:HB3	1:B:1077:GLU:H	1.70	0.56
1:B:1343:GLU:HB3	3:B:404:HOH:O	2.05	0.56
1:A:224:LEU:HD23	1:A:224:LEU:N	2.19	0.56
1:B:1346:PHE:HE2	1:B:1373:LEU:HG	1.72	0.55
1:B:1192:LYS:HD3	3:B:485:HOH:O	2.06	0.55
1:B:1010:TRP:HE1	1:B:1026:GLN:NE2	2.04	0.55
1:A:172:LEU:HB3	1:A:174:GLN:HG3	1.89	0.55
1:B:1087:ASN:HD21	1:B:1142:ILE:H	1.55	0.54
1:B:1248:THR:HG22	3:B:8:HOH:O	2.06	0.54
1:B:1414:PRO:HA	1:B:1419:PHE:CD1	2.42	0.54
1:A:306:LYS:O	1:A:459:HIS:HE1	1.90	0.54
1:B:1014:VAL:CG2	1:B:1029:ALA:HB2	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1248:THR:HB	1:B:1469:TYR:CD1	2.41	0.54
1:A:103:LEU:CD2	1:A:107:ILE:HD11	2.37	0.54
1:A:14:VAL:HG13	1:A:17:LEU:HD21	1.90	0.53
1:B:1227:ASP:HB3	1:B:1284:TYR:CZ	2.44	0.53
1:B:1459:HIS:HD2	3:B:169:HOH:O	1.92	0.53
1:B:1101:LEU:HD22	1:B:1132:GLU:OE2	2.09	0.52
1:B:1146:GLN:NE2	1:B:1158:ALA:H	1.97	0.52
1:A:312:PRO:CA	1:A:367:ILE:HD11	2.39	0.52
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.92	0.52
1:A:452:ARG:HD2	3:B:90:HOH:O	2.09	0.52
1:A:396:ARG:HD2	3:A:641:HOH:O	2.10	0.52
1:B:1020:HIS:CE1	1:B:1087:ASN:HD22	2.27	0.52
1:B:1315:ALA:CB	1:B:1367:ILE:HD13	2.30	0.52
1:A:20:HIS:CD2	1:A:152:THR:OG1	2.59	0.51
1:B:1055:THR:HG23	1:B:1064:THR:HB	1.93	0.51
1:B:1171:LYS:HG2	1:B:1174:GLN:HB2	1.92	0.51
1:A:103:LEU:HD21	1:A:107:ILE:HD11	1.91	0.51
1:B:1055:THR:OG1	1:B:1056:HIS:N	2.43	0.51
1:A:180:ARG:HD2	1:A:188:LYS:HG3	1.92	0.51
1:A:95:ARG:NH2	1:A:107:ILE:O	2.44	0.51
1:A:174:GLN:NE2	1:A:175:TYR:CE2	2.79	0.51
1:B:1273:VAL:HG23	1:B:1275:LYS:HG3	1.92	0.50
1:B:1183:ASN:HB3	3:B:383:HOH:O	2.12	0.50
1:B:1241:GLN:HB3	1:B:1485:TYR:OH	2.11	0.50
1:B:1327:PRO:CG	1:B:1334:GLU:HG2	2.40	0.50
1:B:1009:ALA:HB2	1:B:1214:ILE:HD13	1.94	0.50
1:B:1093:ASP:OD2	1:B:1151:GLU:OE1	2.29	0.50
1:A:40:TYR:CE1	1:A:401:PRO:HB3	2.47	0.49
1:A:14:VAL:HG22	1:A:29:ALA:HB2	1.93	0.49
1:A:206:ALA:O	1:A:210:GLU:HG3	2.12	0.49
1:B:1408:LEU:HD13	1:B:1454:ILE:HG21	1.94	0.49
1:A:357:ALA:HB1	1:A:373:LEU:CD1	2.43	0.49
1:A:312:PRO:HB3	1:A:367:ILE:HD11	1.94	0.49
1:A:472:MET:HE3	1:A:473:MET:N	2.27	0.49
1:B:1279:ILE:HA	1:B:1283:LEU:HB2	1.95	0.49
1:B:1038:VAL:CG1	1:B:1046:VAL:HG21	2.42	0.48
1:B:1257:LYS:HG3	3:B:480:HOH:O	2.12	0.48
1:A:312:PRO:HA	1:A:367:ILE:HD11	1.94	0.48
1:A:75:ASN:HB3	1:A:77:GLU:H	1.78	0.48
1:A:156:ILE:HD13	1:A:156:ILE:H	1.79	0.48
1:B:1106:GLN:NE2	1:B:1124:SER:OG	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:NH1	1:A:373:LEU:HD23	2.30	0.47
1:B:1146:GLN:NE2	1:B:1157:LYS:HB2	2.29	0.47
1:B:1027:MET:HG3	1:B:1137:ARG:CZ	2.44	0.47
1:B:1224:LEU:CD1	3:B:442:HOH:O	2.62	0.47
1:A:20:HIS:CE1	1:A:87:ASN:HD22	2.33	0.47
1:A:54:TRP:HB3	1:A:65:PHE:CD1	2.49	0.47
1:A:257:LYS:HB2	1:A:257:LYS:HE2	1.81	0.47
1:A:246:ILE:HD12	1:A:471:SER:HA	1.97	0.46
1:A:312:PRO:HB3	1:A:367:ILE:CD1	2.46	0.46
1:A:220:ASN:HB3	1:A:472:MET:CE	2.45	0.46
1:A:377:GLU:OE1	1:A:379:SER:N	2.44	0.46
1:A:224:LEU:HD23	1:A:224:LEU:H	1.80	0.46
1:B:1355:SER:O	1:B:1359:ILE:HG13	2.16	0.46
1:B:1121:THR:HG23	3:B:185:HOH:O	2.15	0.46
1:A:361:ARG:HD3	1:A:373:LEU:HD21	1.97	0.46
1:B:1180:ARG:HD2	1:B:1189:PRO:HD2	1.97	0.45
1:B:1223:LEU:HD23	1:B:1224:LEU:HD22	1.97	0.45
1:B:1071:VAL:HG22	1:B:1079:PHE:CB	2.47	0.45
1:B:1332:ILE:HD11	1:B:1365:ARG:NH1	2.30	0.45
1:B:1208:ALA:HB1	1:B:1214:ILE:HD12	1.98	0.45
1:B:1100:TRP:CH2	1:B:1101:LEU:HG	2.51	0.45
1:A:59:ASP:HB3	1:A:61:LYS:H	1.81	0.45
1:A:102:GLU:HB3	1:A:126:TYR:OH	2.16	0.44
1:A:59:ASP:OD2	1:A:61:LYS:HE2	2.17	0.44
1:B:1248:THR:CG2	1:B:1293:LEU:O	2.64	0.44
1:B:1008:THR:CG2	1:B:1216:LEU:O	2.66	0.44
1:A:239:HIS:HD2	3:B:260:HOH:O	1.99	0.44
1:A:220:ASN:HB3	1:A:472:MET:HE3	1.99	0.44
1:B:1306:LYS:O	1:B:1459:HIS:CE1	2.70	0.43
1:A:216:LEU:CD2	1:A:218:TYR:HB2	2.49	0.43
1:A:103:LEU:C	1:A:103:LEU:HD23	2.38	0.43
1:B:1009:ALA:HB2	1:B:1214:ILE:HD11	1.99	0.43
1:B:1188:LYS:HA	1:B:1188:LYS:HD3	1.87	0.43
1:A:441:THR:HG21	1:A:447:ARG:HB2	2.01	0.43
1:B:1427:ASP:OD2	1:B:1461:GLU:OE1	2.37	0.43
1:A:452:ARG:NH2	1:B:1234:GLN:HA	2.34	0.42
1:A:87:ASN:HD21	1:A:142:ILE:H	1.66	0.42
1:A:303:LEU:O	1:A:452:ARG:NH2	2.52	0.42
1:A:80:ASP:HB2	1:A:83:ALA:H	1.83	0.42
1:B:1278:LEU:C	1:B:1278:LEU:HD23	2.40	0.42
1:A:357:ALA:HB1	1:A:373:LEU:HD11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1472:MET:HB2	1:B:1472:MET:HE3	1.73	0.42
1:A:188:LYS:HA	1:A:188:LYS:HD3	1.87	0.42
1:A:106:GLN:HG3	1:A:126:TYR:CG	2.55	0.42
1:B:1181:ASN:C	1:B:1181:ASN:HD22	2.23	0.42
1:A:248:THR:O	1:A:396:ARG:HA	2.19	0.42
1:A:209:PHE:HE2	1:A:238:TYR:CD1	2.38	0.42
1:A:103:LEU:CD2	1:A:103:LEU:C	2.88	0.41
1:A:441:THR:HG21	1:A:447:ARG:CB	2.50	0.41
1:A:181:ASN:ND2	1:A:183:ASN:H	2.18	0.41
1:B:1342:ILE:HG21	1:B:1392:MET:HG3	2.01	0.41
1:B:1441:THR:OG1	1:B:1446:GLN:NE2	2.51	0.41
1:A:246:ILE:HD13	1:A:247:GLU:N	2.35	0.41
1:A:219:GLY:C	1:A:472:MET:CE	2.84	0.41
1:A:245:PRO:O	1:B:1244:GLN:NE2	2.53	0.41
1:A:472:MET:CA	1:A:472:MET:CE	2.89	0.41
1:A:38:VAL:CG1	1:A:46:VAL:HG21	2.46	0.41
1:A:306:LYS:HA	1:A:307:PRO:HD3	1.94	0.41
1:A:332:ILE:HG12	1:A:370:ASP:HB2	2.02	0.41
1:A:361:ARG:HD3	1:A:373:LEU:HD23	2.01	0.40
1:A:242:LEU:O	1:B:1297:SER:HA	2.21	0.40
1:B:1334:GLU:O	1:B:1334:GLU:HG3	2.21	0.40
1:A:312:PRO:CB	1:A:367:ILE:HD11	2.50	0.40
1:B:1180:ARG:HD2	1:B:1188:LYS:HG3	2.03	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	495/502 (99%)	483 (98%)	11 (2%)	1 (0%)	52 43
1	B	494/502 (98%)	480 (97%)	13 (3%)	1 (0%)	52 43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	989/1004 (98%)	963 (97%)	24 (2%)	2 (0%)	52 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	LYS
1	B	1378	GLU

### 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	422/425 (99%)	361 (86%)	61 (14%)	4 0
1	B	421/425 (99%)	362 (86%)	59 (14%)	4 1
All	All	843/850 (99%)	723 (86%)	120 (14%)	4 1

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	12	VAL
1	A	14	VAL
1	A	38	VAL
1	A	46	VAL
1	A	52	LYS
1	A	55	THR
1	A	56	HIS
1	A	58	GLU
1	A	59	ASP
1	A	62	THR
1	A	71	VAL
1	A	82	GLU
1	A	95	ARG
1	A	97	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	101	LEU
1	A	103	LEU
1	A	109	ASP
1	A	111	LYS
1	A	115	LYS
1	A	127	TYR
1	A	137	ARG
1	A	148	LYS
1	A	151	GLU
1	A	156	ILE
1	A	167	LEU
1	A	171	LYS
1	A	174	GLN
1	A	179	VAL
1	A	181	ASN
1	A	182	GLU
1	A	188	LYS
1	A	216	LEU
1	A	220	ASN
1	A	246	ILE
1	A	248	THR
1	A	249	VAL
1	A	253	LEU
1	A	309	GLN
1	A	319	LEU
1	A	330	LYS
1	A	347	ILE
1	A	352	LEU
1	A	367	ILE
1	A	371	VAL
1	A	377	GLU
1	A	379	SER
1	A	380	SER
1	A	382	TYR
1	A	396	ARG
1	A	420	GLN
1	A	427	ASP
1	A	438	VAL
1	A	439	LEU
1	A	441	THR
1	A	450	LEU
1	A	452	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	472	MET
1	A	476	SER
1	A	480	LEU
1	B	1008	THR
1	B	1014	VAL
1	B	1023	THR
1	B	1024	PRO
1	B	1038	VAL
1	B	1046	VAL
1	B	1055	THR
1	B	1056	HIS
1	B	1062	THR
1	B	1071	VAL
1	B	1080	ASP
1	B	1096	GLN
1	B	1097	ARG
1	B	1101	LEU
1	B	1103	LEU
1	B	1115	LYS
1	B	1123	LYS
1	B	1127	TYR
1	B	1137	ARG
1	B	1138	PRO
1	B	1167	LEU
1	B	1172	LEU
1	B	1179	VAL
1	B	1181	ASN
1	B	1182	GLU
1	B	1188	LYS
1	B	1214	ILE
1	B	1216	LEU
1	B	1220	ASN
1	B	1223	LEU
1	B	1242	LEU
1	B	1248	THR
1	B	1253	LEU
1	B	1276	LYS
1	B	1309	GLN
1	B	1319	LEU
1	B	1334	GLU
1	B	1343	GLU
1	B	1344	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1345	SER
1	B	1347	ILE
1	B	1352	LEU
1	B	1353	SER
1	B	1367	ILE
1	B	1371	VAL
1	B	1373	LEU
1	B	1378	GLU
1	B	1380	SER
1	B	1384	ARG
1	B	1393	ILE
1	B	1415	SER
1	B	1439	LEU
1	B	1450	LEU
1	B	1465	LEU
1	B	1470	ILE
1	B	1476	SER
1	B	1479	GLU
1	B	1482	ASN
1	B	1498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	26	GLN
1	A	87	ASN
1	A	105	ASN
1	A	106	GLN
1	A	146	GLN
1	A	174	GLN
1	A	181	ASN
1	A	220	ASN
1	A	239	HIS
1	A	244	GLN
1	A	288	GLN
1	A	309	GLN
1	A	420	GLN
1	A	459	HIS
1	A	496	GLN
1	B	1013	ASN
1	B	1020	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1026	GLN
1	B	1087	ASN
1	B	1106	GLN
1	B	1146	GLN
1	B	1149	ASN
1	B	1181	ASN
1	B	1197	ASN
1	B	1220	ASN
1	B	1239	HIS
1	B	1288	GLN
1	B	1302	ASN
1	B	1309	GLN
1	B	1336	ASN
1	B	1385	GLN
1	B	1420	GLN
1	B	1423	GLN
1	B	1446	GLN
1	B	1459	HIS
1	B	1482	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	497/502 (99%)	0.15	18 (3%)	46 57	13, 25, 42, 54	0
1	B	496/502 (98%)	0.13	15 (3%)	54 64	14, 24, 42, 53	0
All	All	993/1004 (98%)	0.14	33 (3%)	50 61	13, 24, 42, 54	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	TYR	5.3
1	B	1058	GLU	3.9
1	B	1351	ALA	3.8
1	B	1378	GLU	3.8
1	A	149	ASN	3.7
1	A	4	ASP	3.5
1	B	1221	GLU	3.3
1	A	386	ARG	3.3
1	B	1328	ALA	3.3
1	B	1382	TYR	3.1
1	A	442	HIS	3.1
1	A	56	HIS	3.0
1	A	499	PRO	3.0
1	B	1341	ARG	2.9
1	B	1347	ILE	2.8
1	A	329	GLY	2.8
1	B	1056	HIS	2.8
1	A	148	LYS	2.7
1	A	328	ALA	2.7
1	B	1349	THR	2.6
1	B	1281	ASN	2.6
1	A	115	LYS	2.6
1	A	150	HIS	2.5
1	B	1095	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	169	GLU	2.4
1	A	37	LEU	2.4
1	A	58	GLU	2.3
1	B	1023	THR	2.3
1	B	1188	LYS	2.3
1	A	500	VAL	2.1
1	A	114	SER	2.1
1	B	1386	ARG	2.0
1	A	157	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NI	B	1503	1/1	0.99	0.05	-	36,36,36,36	0
2	NI	A	503	1/1	1.00	0.02	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.