Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 05:33 AM EDT

PDB ID	:	1NB4
Title	:	HC-J4 RNA polymerase apo-form
Authors	:	Jaeger, J.; O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.
Deposited on	:	2002-12-02
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

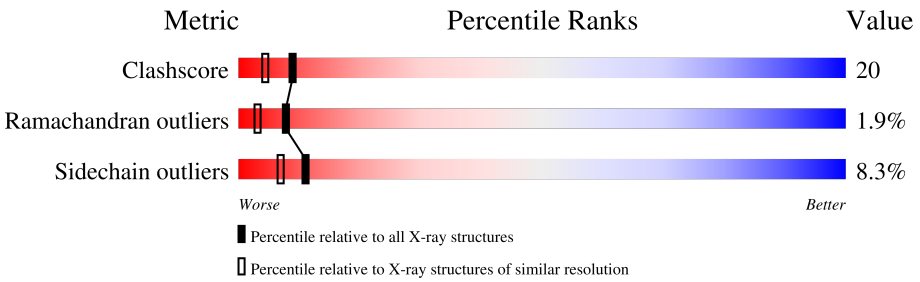
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	570	68% 28% • ••
1	B	570	69% 22% 8% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9554 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 polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	566	4388	2763	777	816	32	0	0	0
1	B	565	4383	2760	776	815	32	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	344	344	344	0	0
2	B	439	439	439	0	0

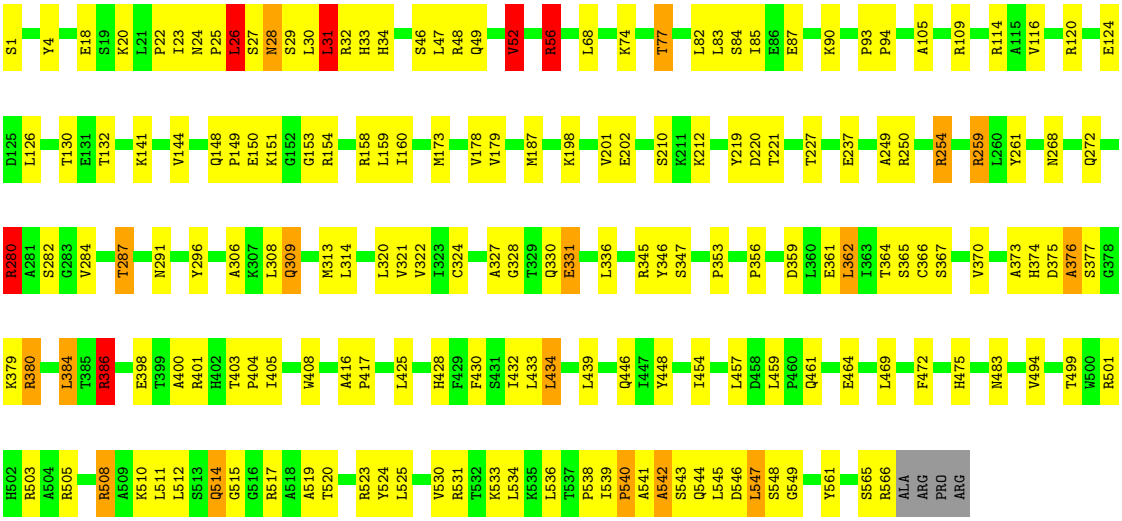
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

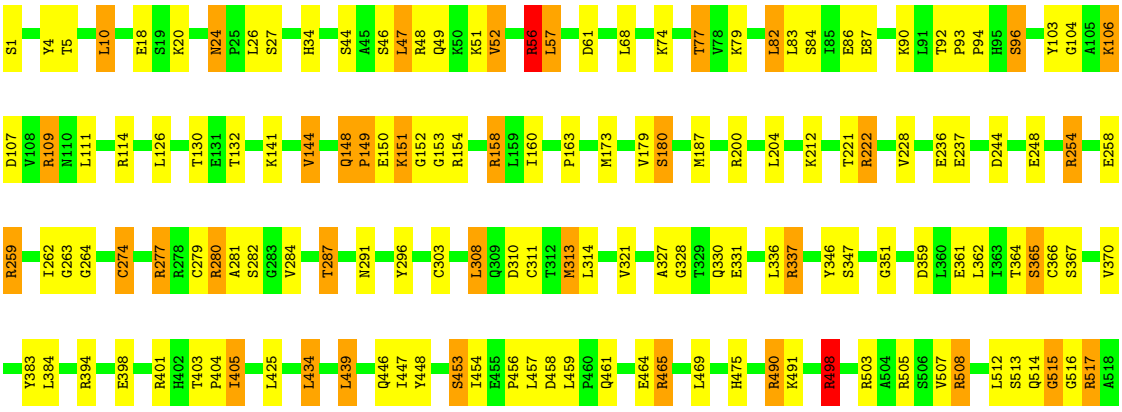
• Molecule 1: polyprotein

Chain A:



• Molecule 1: polyprotein

Chain B:



A519
R523
V530
R531
L534
K535
P538
I539
P540
A541
A542
S543
Q544
L545
D546
L547
S548
G549
W550
S556
G557
G558
D559
H562
S563
L564
S565
ARG
ALA
ARG
PRO
ARG

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.69Å 108.71Å 135.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (55.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9554	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

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	0.86	2/4484 (0.0%)	0.95	11/6087 (0.2%)
1	B	0.99	3/4479 (0.1%)	0.99	13/6080 (0.2%)
All	All	0.93	5/8963 (0.1%)	0.97	24/12167 (0.2%)

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
1	B	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	CYS	CB-SG	-9.77	1.65	1.82
1	B	179	VAL	CB-CG1	-6.55	1.39	1.52
1	B	180	SER	CB-OG	-6.21	1.34	1.42
1	A	52	VAL	CB-CG1	-5.41	1.41	1.52
1	A	261	TYR	CD2-CE2	5.16	1.47	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	B	280	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	A	280	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	280	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	B	259	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	B	56	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	259	ARG	NE-CZ-NH2	-8.52	116.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	508	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	114	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	A	31	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	254	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	254	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	56	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	250	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	475	HIS	N-CA-C	5.84	126.78	111.00
1	B	56	ARG	CG-CD-NE	-5.80	99.61	111.80
1	B	498	ARG	CG-CD-NE	5.60	123.55	111.80
1	B	558	GLY	N-CA-C	-5.48	99.41	113.10
1	A	384	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	386	ARG	CG-CD-NE	-5.34	100.59	111.80
1	A	254	ARG	CG-CD-NE	-5.32	100.63	111.80
1	B	109	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	B	434	LEU	CA-CB-CG	5.07	126.95	115.30
1	B	254	ARG	CG-CD-NE	-5.04	101.23	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	TYR	Sidechain
1	B	383	TYR	Sidechain
1	B	498	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	4388	0	4383	184	0
1	B	4383	0	4381	173	0
2	A	344	0	0	35	0
2	B	439	0	0	42	0
All	All	9554	0	8764	356	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 20.

All (356) 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:130:THR:HB	2:B:800:HOH:O	1.31	1.25
1:B:277:ARG:HH11	1:B:277:ARG:HB3	1.14	1.10
1:A:547:LEU:HD12	1:A:565:SER:H	1.06	1.08
1:B:109:ARG:NH1	1:B:109:ARG:HB2	1.72	1.05
1:A:327:ALA:O	1:A:331:GLU:HG3	1.61	1.01
1:A:20:LYS:O	1:A:22:PRO:HD3	1.65	0.97
1:B:277:ARG:HH11	1:B:277:ARG:CB	1.77	0.96
1:A:373:ALA:HB1	2:A:872:HOH:O	1.66	0.95
1:B:461:GLN:HB3	1:B:542:ALA:HA	1.49	0.94
1:B:337:ARG:HG3	2:B:977:HOH:O	1.67	0.94
1:A:24:ASN:ND2	1:A:27:SER:H	1.66	0.93
1:B:200:ARG:NH1	1:B:204:LEU:HD11	1.83	0.93
1:B:200:ARG:NE	2:B:749:HOH:O	2.01	0.92
1:A:405:ILE:HD11	1:A:446:GLN:HG2	1.49	0.92
1:A:56:ARG:NH2	2:A:643:HOH:O	2.08	0.87
1:A:56:ARG:NE	2:A:643:HOH:O	2.08	0.87
1:A:547:LEU:HD12	1:A:565:SER:N	1.90	0.87
1:B:277:ARG:CZ	2:B:628:HOH:O	2.21	0.87
1:B:277:ARG:HB3	1:B:277:ARG:NH1	1.88	0.86
1:A:24:ASN:ND2	1:A:27:SER:N	2.24	0.86
1:A:141:LYS:HE3	1:A:158:ARG:NH2	1.89	0.86
1:B:200:ARG:CZ	2:B:749:HOH:O	2.24	0.85
1:A:84:SER:OG	1:A:87:GLU:HG3	1.76	0.85
1:A:24:ASN:HD22	1:A:27:SER:HB2	1.40	0.84
1:B:327:ALA:O	1:B:331:GLU:HG3	1.77	0.84
1:B:264:GLY:N	1:B:277:ARG:HH12	1.76	0.84
1:A:124:GLU:HG3	2:A:881:HOH:O	1.77	0.83
1:B:61:ASP:CG	2:B:588:HOH:O	2.17	0.83
1:A:547:LEU:CD1	1:A:565:SER:H	1.91	0.82
1:A:105:ALA:O	1:A:109:ARG:HG3	1.80	0.81
1:A:148:GLN:HG2	1:A:150:GLU:H	1.45	0.81
1:B:18:GLU:HG2	1:B:401:ARG:NH1	1.95	0.81
1:A:56:ARG:HB2	1:A:56:ARG:NH1	1.95	0.80
1:B:141:LYS:NZ	1:B:158:ARG:HH12	1.81	0.79
1:B:464:GLU:HG3	1:B:469:LEU:HD12	1.63	0.79
1:B:222:ARG:HG3	1:B:351:GLY:HA2	1.65	0.79
1:A:24:ASN:HD22	1:A:27:SER:CB	1.95	0.78
1:A:56:ARG:HB2	1:A:56:ARG:HH11	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:HB2	1:B:109:ARG:HH11	1.46	0.78
1:A:268:ASN:HD21	1:A:272:GLN:HE21	1.29	0.77
1:A:56:ARG:CZ	2:A:643:HOH:O	2.30	0.76
1:B:18:GLU:HG2	1:B:401:ARG:CZ	2.15	0.76
1:B:148:GLN:HE21	1:B:153:GLY:HA3	1.49	0.75
1:B:132:THR:O	1:B:259:ARG:CD	2.34	0.75
1:A:280:ARG:HD2	1:A:291:ASN:OD1	1.87	0.74
1:A:359:ASP:HB3	1:A:362:LEU:HD22	1.68	0.74
1:B:160:ILE:HD12	1:B:282:SER:OG	1.87	0.74
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.53	0.74
1:B:403:THR:HB	1:B:404:PRO:HD2	1.69	0.74
1:B:109:ARG:HH11	1:B:109:ARG:CB	2.01	0.74
1:B:132:THR:O	1:B:259:ARG:HD2	1.88	0.73
1:A:22:PRO:HB2	2:A:619:HOH:O	1.88	0.73
1:A:475:HIS:N	2:A:872:HOH:O	2.20	0.73
1:A:132:THR:O	1:A:259:ARG:HD2	1.88	0.73
1:B:548:SER:O	1:B:550:TRP:N	2.22	0.73
1:A:24:ASN:HD22	1:A:27:SER:N	1.84	0.72
1:B:558:GLY:O	2:B:591:HOH:O	2.06	0.72
1:B:152:GLY:HA2	2:B:644:HOH:O	1.88	0.72
1:A:28:ASN:HB2	2:A:774:HOH:O	1.90	0.72
1:B:361:GLU:HB2	2:B:948:HOH:O	1.90	0.72
1:A:198:LYS:O	1:A:201:VAL:HG12	1.90	0.71
1:A:132:THR:O	1:A:259:ARG:CD	2.38	0.71
1:B:277:ARG:NE	2:B:628:HOH:O	2.21	0.70
1:A:26:LEU:O	1:A:29:SER:HB3	1.90	0.70
1:A:148:GLN:OE1	1:A:153:GLY:HA3	1.89	0.70
1:B:154:ARG:HD3	2:B:958:HOH:O	1.91	0.70
1:B:130:THR:HG21	2:B:680:HOH:O	1.92	0.70
1:B:490:ARG:HE	1:B:490:ARG:HA	1.57	0.70
1:B:534:LEU:HD12	1:B:535:LYS:N	2.07	0.70
1:B:465:ARG:HD3	1:B:543:SER:HA	1.74	0.69
1:A:178:VAL:HG23	2:A:649:HOH:O	1.92	0.69
1:A:24:ASN:HD22	1:A:27:SER:H	1.36	0.69
1:B:200:ARG:HH12	1:B:204:LEU:HD11	1.56	0.69
1:A:501:ARG:HB3	2:A:794:HOH:O	1.92	0.69
1:A:148:GLN:CD	1:A:150:GLU:HG2	2.12	0.68
1:A:361:GLU:HG3	1:A:370:VAL:O	1.93	0.68
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.76	0.68
1:B:200:ARG:NH2	2:B:749:HOH:O	2.27	0.67
1:A:85:ILE:N	1:A:173:MET:HE3	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:HA	2:B:996:HOH:O	1.94	0.66
1:A:547:LEU:N	1:A:547:LEU:HD23	2.11	0.66
1:A:284:VAL:CG2	1:A:287:THR:HG22	2.26	0.66
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.25	0.66
1:A:538:PRO:HB2	2:A:792:HOH:O	1.95	0.66
1:B:200:ARG:HH11	1:B:204:LEU:HD11	1.61	0.66
1:A:398:GLU:HG2	1:A:403:THR:HG21	1.77	0.66
1:A:90:LYS:HG2	2:A:891:HOH:O	1.96	0.66
1:B:277:ARG:HH11	1:B:277:ARG:CG	2.07	0.66
1:A:1:SER:O	1:A:56:ARG:NH1	2.29	0.65
1:A:284:VAL:HG23	1:A:287:THR:HG22	1.79	0.65
1:B:303:CYS:SG	1:B:313:MET:CE	2.85	0.65
1:B:534:LEU:HD12	1:B:534:LEU:C	2.18	0.64
1:A:539:ILE:HG23	1:A:540:PRO:HD2	1.80	0.63
1:A:461:GLN:HG3	1:A:542:ALA:HB2	1.79	0.63
1:A:74:LYS:O	1:A:77:THR:HB	1.97	0.63
1:A:148:GLN:NE2	1:A:150:GLU:HG2	2.12	0.63
1:B:109:ARG:NH1	1:B:109:ARG:CB	2.53	0.63
1:A:353:PRO:HG3	2:A:740:HOH:O	1.97	0.63
1:A:401:ARG:HG3	2:A:884:HOH:O	1.97	0.63
1:B:46:SER:HA	1:B:49:GLN:HE21	1.62	0.63
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.80	0.62
1:B:361:GLU:HG3	1:B:370:VAL:O	2.00	0.62
1:B:359:ASP:HB3	1:B:362:LEU:HD22	1.80	0.62
1:A:439:LEU:N	1:A:439:LEU:HD22	2.15	0.61
1:A:520:THR:HA	1:A:523:ARG:HD2	1.82	0.61
1:B:158:ARG:HH11	1:B:158:ARG:CB	2.13	0.61
1:B:132:THR:O	1:B:259:ARG:HD3	2.00	0.61
1:A:28:ASN:OD1	1:A:34:HIS:CE1	2.54	0.61
1:B:547:LEU:H	1:B:547:LEU:CD1	2.14	0.61
1:A:237:GLU:OE2	1:A:254:ARG:HD2	2.01	0.61
1:A:148:GLN:CG	1:A:150:GLU:HG2	2.31	0.60
1:A:346:TYR:O	1:A:347:SER:HB3	1.99	0.60
1:A:539:ILE:CG2	1:A:540:PRO:HD2	2.31	0.60
1:A:524:TYR:CD2	1:A:536:LEU:HD22	2.36	0.60
1:B:57:LEU:HD13	2:B:717:HOH:O	2.00	0.60
1:B:505:ARG:HH21	1:B:531:ARG:NE	1.99	0.60
1:A:365:SER:O	1:A:366:CYS:HB2	2.01	0.60
1:B:150:GLU:H	1:B:150:GLU:CD	2.03	0.60
1:B:303:CYS:SG	1:B:313:MET:HE3	2.42	0.60
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LYS:O	1:A:201:VAL:CG1	2.50	0.59
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.32	0.59
1:B:547:LEU:CD1	1:B:547:LEU:N	2.65	0.59
1:B:48:ARG:CZ	1:B:51:LYS:NZ	2.66	0.59
1:B:490:ARG:HA	1:B:490:ARG:NE	2.17	0.59
1:A:30:LEU:O	1:A:494:VAL:HG22	2.03	0.58
1:A:179:VAL:HG13	2:A:591:HOH:O	2.03	0.58
1:A:33:HIS:CE1	1:B:212:LYS:HE2	2.39	0.58
1:A:377:SER:HB3	2:A:771:HOH:O	2.03	0.58
1:A:405:ILE:CD1	1:A:446:GLN:HG2	2.29	0.58
1:A:24:ASN:O	2:A:774:HOH:O	2.17	0.58
1:B:464:GLU:HG3	1:B:469:LEU:CD1	2.32	0.58
1:A:268:ASN:HD21	1:A:272:GLN:NE2	2.02	0.58
1:B:277:ARG:NH2	2:B:628:HOH:O	2.31	0.57
1:A:540:PRO:HG2	1:A:541:ALA:H	1.69	0.57
1:B:141:LYS:HZ2	1:B:158:ARG:HH12	1.50	0.57
1:A:379:LYS:C	2:A:776:HOH:O	2.43	0.57
1:A:511:LEU:O	1:A:514:GLN:HB2	2.05	0.57
1:B:82:LEU:HD12	1:B:82:LEU:O	2.03	0.57
1:B:187:MET:HE3	1:B:296:TYR:CD1	2.38	0.57
1:B:248:GLU:HG3	2:B:577:HOH:O	2.04	0.57
1:A:24:ASN:HB2	1:A:400:ALA:HB2	1.86	0.57
1:B:10:LEU:H	1:B:10:LEU:HD22	1.68	0.57
1:B:46:SER:HA	1:B:49:GLN:NE2	2.19	0.57
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.87	0.57
1:A:405:ILE:HD11	1:A:446:GLN:CG	2.29	0.56
1:A:512:LEU:C	1:A:514:GLN:H	2.08	0.56
1:A:24:ASN:HB2	1:A:400:ALA:CB	2.34	0.56
1:A:116:VAL:O	1:A:120:ARG:HG3	2.05	0.56
1:A:34:HIS:CD2	2:A:800:HOH:O	2.58	0.56
1:B:150:GLU:HA	2:B:914:HOH:O	2.06	0.56
1:B:503:ARG:O	1:B:507:VAL:HG23	2.06	0.56
1:B:200:ARG:HD3	1:B:384:LEU:HD11	1.88	0.56
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.21	0.56
1:B:331:GLU:CD	1:B:331:GLU:H	2.07	0.55
1:B:465:ARG:HE	1:B:546:ASP:CB	2.19	0.55
1:A:24:ASN:OD1	1:A:25:PRO:HD2	2.07	0.55
1:B:86:GLU:HG3	1:B:111:LEU:HD11	1.89	0.55
1:B:263:GLY:C	1:B:277:ARG:HH12	2.09	0.55
1:B:56:ARG:NH2	1:B:228:VAL:O	2.40	0.54
1:A:454:ILE:HA	1:A:566:ARG:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:N	1:A:461:GLN:OE1	2.39	0.54
1:B:457:LEU:HD13	1:B:517:ARG:HH11	1.72	0.54
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.22	0.54
1:A:364:THR:HG22	2:A:785:HOH:O	2.07	0.54
1:B:541:ALA:O	1:B:542:ALA:O	2.25	0.54
1:A:548:SER:OG	1:A:549:GLY:N	2.40	0.54
1:A:280:ARG:CD	1:A:291:ASN:OD1	2.55	0.54
1:B:465:ARG:HH21	1:B:546:ASP:CB	2.21	0.54
1:A:28:ASN:CB	2:A:774:HOH:O	2.53	0.53
1:B:547:LEU:H	1:B:547:LEU:HD13	1.72	0.53
1:B:491:LYS:HE3	2:B:663:HOH:O	2.08	0.53
1:B:280:ARG:HD2	1:B:291:ASN:OD1	2.09	0.53
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.91	0.53
1:A:374:HIS:HA	2:A:776:HOH:O	2.08	0.53
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.91	0.53
1:B:457:LEU:CD1	1:B:517:ARG:NH1	2.72	0.53
1:A:336:LEU:HD22	1:A:356:PRO:HD3	1.91	0.53
1:A:85:ILE:HA	1:A:173:MET:HE3	1.90	0.53
1:A:24:ASN:ND2	1:A:27:SER:HB2	2.16	0.52
1:B:405:ILE:HD11	1:B:446:GLN:HG2	1.91	0.52
1:A:33:HIS:HE1	2:A:689:HOH:O	1.91	0.51
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.40	0.51
1:A:154:ARG:HG3	1:A:154:ARG:NH1	2.24	0.51
1:A:85:ILE:CA	1:A:173:MET:HE3	2.41	0.51
1:A:94:PRO:HA	1:A:109:ARG:HD2	1.93	0.51
1:A:510:LYS:HE2	2:A:787:HOH:O	2.10	0.51
1:A:24:ASN:HD22	1:A:27:SER:CA	2.23	0.51
1:A:531:ARG:NH2	2:A:865:HOH:O	2.43	0.51
1:B:130:THR:CB	2:B:800:HOH:O	2.13	0.51
1:B:337:ARG:CG	2:B:977:HOH:O	2.43	0.51
1:B:74:LYS:O	1:B:77:THR:HB	2.08	0.51
1:A:34:HIS:HD2	2:A:800:HOH:O	1.94	0.51
1:B:464:GLU:OE1	1:B:469:LEU:HD11	2.11	0.51
1:A:149:PRO:HB2	1:A:150:GLU:OE2	2.11	0.50
1:B:24:ASN:ND2	1:B:26:LEU:H	2.09	0.50
1:B:453:SER:HB2	1:B:563:SER:CB	2.42	0.50
1:A:403:THR:OG1	1:A:404:PRO:HD2	2.11	0.50
1:A:547:LEU:HG	1:A:565:SER:HA	1.94	0.50
1:A:284:VAL:O	1:A:287:THR:HG23	2.11	0.50
1:A:375:ASP:N	2:A:776:HOH:O	2.17	0.50
1:A:4:TYR:CE1	1:A:52:VAL:HG13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:HIS:CD2	2:B:821:HOH:O	2.65	0.50
1:A:439:LEU:H	1:A:439:LEU:CD2	2.25	0.49
1:B:93:PRO:HG2	1:B:96:SER:OG	2.12	0.49
1:B:453:SER:H	1:B:563:SER:HA	1.77	0.49
1:B:547:LEU:N	1:B:547:LEU:HD12	2.25	0.49
1:A:132:THR:O	1:A:259:ARG:HD3	2.12	0.49
1:A:505:ARG:NH2	1:A:531:ARG:HE	2.10	0.49
1:B:327:ALA:C	1:B:331:GLU:HG3	2.33	0.49
1:A:28:ASN:N	2:A:774:HOH:O	2.46	0.49
1:A:160:ILE:HD12	1:A:282:SER:OG	2.12	0.49
1:A:28:ASN:OD1	1:A:34:HIS:HE1	1.96	0.49
1:B:10:LEU:HD22	1:B:10:LEU:N	2.27	0.49
1:A:31:LEU:O	1:A:31:LEU:HD23	2.12	0.49
1:A:519:ALA:O	1:A:523:ARG:HG3	2.12	0.49
1:A:83:LEU:HB2	1:A:173:MET:HA	1.94	0.49
1:B:79:LYS:HG3	1:B:244:ASP:HB3	1.93	0.49
1:B:548:SER:O	1:B:549:GLY:C	2.51	0.49
1:A:508:ARG:NH2	1:A:530:VAL:HG11	2.28	0.48
1:B:346:TYR:O	1:B:347:SER:HB3	2.13	0.48
1:B:556:SER:C	1:B:558:GLY:H	2.16	0.48
1:B:254:ARG:NH2	1:B:258:GLU:CG	2.76	0.48
1:A:26:LEU:HD11	1:A:432:ILE:HD12	1.95	0.48
1:B:153:GLY:HA2	2:B:982:HOH:O	2.12	0.48
1:B:337:ARG:HA	1:B:337:ARG:HE	1.78	0.48
1:A:56:ARG:HH11	1:A:56:ARG:CB	2.21	0.48
1:A:439:LEU:N	1:A:439:LEU:CD2	2.76	0.48
1:A:398:GLU:HG2	1:A:403:THR:CG2	2.44	0.48
1:B:48:ARG:CZ	1:B:51:LYS:HZ1	2.26	0.48
1:B:222:ARG:HG3	1:B:351:GLY:CA	2.42	0.47
1:B:109:ARG:NE	2:B:915:HOH:O	2.42	0.47
1:B:34:HIS:HD2	2:B:794:HOH:O	1.95	0.47
1:B:4:TYR:CE1	1:B:52:VAL:HG13	2.50	0.47
1:B:461:GLN:HB3	1:B:542:ALA:CA	2.32	0.47
1:B:505:ARG:NH1	2:B:613:HOH:O	2.47	0.47
1:A:284:VAL:HG22	1:A:287:THR:HG22	1.96	0.47
1:B:277:ARG:NH1	1:B:277:ARG:CG	2.74	0.47
1:B:237:GLU:OE2	1:B:254:ARG:HD2	2.14	0.47
1:A:328:GLY:HA3	1:A:331:GLU:HG2	1.97	0.47
1:B:446:GLN:C	1:B:447:ILE:HD12	2.36	0.47
1:B:200:ARG:NH1	2:B:635:HOH:O	2.47	0.47
1:A:220:ASP:HB3	2:A:867:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD11	1:B:514:GLN:NE2	2.30	0.46
1:A:379:LYS:O	1:A:380:ARG:C	2.53	0.46
1:B:457:LEU:HD12	1:B:517:ARG:NH1	2.31	0.46
1:B:523:ARG:HD3	1:B:534:LEU:HD21	1.97	0.46
1:A:375:ASP:O	1:A:376:ALA:C	2.53	0.46
1:B:284:VAL:HG23	1:B:287:THR:HG22	1.98	0.46
1:A:439:LEU:HD22	1:A:439:LEU:H	1.80	0.46
1:A:457:LEU:HB3	1:A:517:ARG:HB3	1.98	0.46
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.98	0.46
1:A:198:LYS:HB2	2:A:672:HOH:O	2.15	0.46
1:B:280:ARG:CD	1:B:291:ASN:OD1	2.63	0.46
1:A:227:THR:HB	1:A:347:SER:O	2.17	0.45
1:B:284:VAL:CG2	1:B:287:THR:HG22	2.46	0.45
1:B:56:ARG:NH2	1:B:279:CYS:HB3	2.31	0.45
1:B:82:LEU:HD12	1:B:82:LEU:C	2.36	0.45
1:B:439:LEU:O	1:B:456:PRO:HG2	2.16	0.45
1:B:464:GLU:CD	1:B:469:LEU:HD11	2.36	0.45
1:B:130:THR:CG2	2:B:680:HOH:O	2.60	0.45
1:A:503:ARG:HG2	1:A:503:ARG:HH11	1.82	0.45
1:A:533:LYS:HD3	2:A:763:HOH:O	2.15	0.45
1:B:114:ARG:HG2	2:B:830:HOH:O	2.17	0.45
1:B:144:VAL:HG22	1:B:394:ARG:HG2	1.98	0.45
1:A:524:TYR:CG	1:A:536:LEU:HD22	2.51	0.45
1:B:24:ASN:ND2	1:B:26:LEU:N	2.64	0.45
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.32	0.45
1:A:464:GLU:HG3	1:A:469:LEU:CD1	2.47	0.45
1:A:503:ARG:CZ	2:A:906:HOH:O	2.65	0.45
1:B:365:SER:O	1:B:366:CYS:HB2	2.16	0.45
1:B:277:ARG:HE	1:B:281:ALA:HB2	1.82	0.45
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.85	0.44
1:A:428:HIS:O	1:A:432:ILE:HG12	2.17	0.44
1:B:517:ARG:NH1	1:B:517:ARG:HG3	2.32	0.44
1:B:1:SER:HA	2:B:908:HOH:O	2.17	0.44
1:B:490:ARG:NE	1:B:490:ARG:CA	2.79	0.44
1:A:24:ASN:CB	1:A:400:ALA:HB2	2.46	0.44
1:A:46:SER:HA	1:A:49:GLN:HE21	1.81	0.44
1:B:458:ASP:OD1	2:B:974:HOH:O	2.21	0.44
1:B:236:GLU:OE2	2:B:600:HOH:O	2.20	0.44
1:A:367:SER:O	1:A:386:ARG:HB2	2.18	0.44
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.81	0.44
1:B:48:ARG:CZ	1:B:51:LYS:HZ3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:SER:OG	1:B:559:ASP:OD1	2.36	0.44
1:A:32:ARG:HD2	2:A:825:HOH:O	2.17	0.44
1:A:514:GLN:HE21	1:A:514:GLN:HB3	1.56	0.44
1:B:394:ARG:O	1:B:398:GLU:HG3	2.18	0.44
1:A:26:LEU:HD21	1:A:432:ILE:HD11	2.00	0.43
1:A:398:GLU:OE2	1:A:408:TRP:HD1	2.01	0.43
1:A:542:ALA:C	1:A:544:GLN:H	2.20	0.43
1:B:328:GLY:O	1:B:331:GLU:HG2	2.18	0.43
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.99	0.43
1:B:314:LEU:HD12	1:B:314:LEU:HA	1.84	0.43
1:B:448:TYR:HB2	2:B:747:HOH:O	2.19	0.43
1:A:201:VAL:HG13	1:A:202:GLU:N	2.33	0.43
1:A:154:ARG:HH11	1:A:154:ARG:CG	2.27	0.43
1:B:24:ASN:HD22	1:B:27:SER:H	1.67	0.43
1:B:150:GLU:O	1:B:151:LYS:C	2.57	0.43
1:A:31:LEU:HD23	1:A:31:LEU:C	2.38	0.43
1:B:5:THR:HG22	2:B:851:HOH:O	2.18	0.43
1:B:530:VAL:HG11	2:B:742:HOH:O	2.19	0.43
1:B:457:LEU:HD12	1:B:517:ARG:HH12	1.83	0.42
1:A:472:PHE:HE2	1:A:525:LEU:HD23	1.83	0.42
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.83	0.42
1:A:308:LEU:N	1:A:308:LEU:HD12	2.34	0.42
1:A:430:PHE:O	1:A:434:LEU:HB2	2.19	0.42
1:A:524:TYR:CE2	1:A:536:LEU:HB3	2.55	0.42
1:B:447:ILE:HD12	1:B:447:ILE:N	2.34	0.42
1:B:434:LEU:CD1	1:B:514:GLN:NE2	2.82	0.42
1:B:453:SER:C	1:B:454:ILE:HG12	2.39	0.42
1:A:306:ALA:HB3	1:A:308:LEU:CD1	2.47	0.42
1:B:187:MET:HE1	1:B:296:TYR:HB2	2.01	0.42
1:A:148:GLN:HG2	1:A:150:GLU:HG2	2.01	0.42
1:B:83:LEU:HB2	1:B:173:MET:HA	2.00	0.42
1:A:148:GLN:HG2	1:A:150:GLU:N	2.25	0.42
1:A:416:ALA:N	1:A:417:PRO:HD3	2.35	0.42
1:A:483:ASN:HD22	1:A:483:ASN:HA	1.65	0.41
1:A:306:ALA:CB	1:A:308:LEU:CD1	2.97	0.41
1:A:499:THR:HG23	2:B:723:HOH:O	2.20	0.41
1:B:153:GLY:CA	2:B:982:HOH:O	2.68	0.41
1:B:512:LEU:O	1:B:513:SER:C	2.57	0.41
1:B:531:ARG:NH2	2:B:890:HOH:O	2.32	0.41
1:A:20:LYS:O	1:A:22:PRO:CD	2.53	0.41
1:B:92:THR:HA	1:B:93:PRO:HD2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.87	0.41
1:B:457:LEU:HD13	1:B:517:ARG:NH1	2.34	0.41
1:A:148:GLN:HG3	1:A:149:PRO:HD2	2.01	0.41
1:A:464:GLU:OE2	1:A:538:PRO:HA	2.21	0.41
1:B:106:LYS:HB3	2:B:932:HOH:O	2.20	0.41
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.41
1:B:86:GLU:OE2	1:B:90:LYS:HE3	2.20	0.41
1:B:158:ARG:HD3	2:B:883:HOH:O	2.20	0.41
1:A:22:PRO:CD	2:A:653:HOH:O	2.69	0.41
1:A:26:LEU:CD1	1:A:432:ILE:HD12	2.50	0.41
1:A:187:MET:HE3	1:A:296:TYR:CD1	2.56	0.41
1:B:461:GLN:OE1	1:B:461:GLN:N	2.40	0.41
1:A:219:TYR:HE2	1:A:221:THR:HG22	1.85	0.41
1:A:346:TYR:O	1:A:347:SER:CB	2.67	0.41
1:B:150:GLU:CA	2:B:914:HOH:O	2.68	0.41
1:A:93:PRO:HB3	1:A:561:TYR:HB2	2.03	0.41
1:A:508:ARG:CZ	1:A:530:VAL:CG1	2.97	0.41
1:B:516:GLY:O	1:B:517:ARG:C	2.58	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.21	0.40
1:B:104:GLY:O	1:B:107:ASP:HB2	2.20	0.40
1:A:308:LEU:N	1:A:308:LEU:CD1	2.83	0.40
1:A:27:SER:HB3	2:A:650:HOH:O	2.20	0.40
1:A:309:GLN:O	1:A:324:CYS:HB2	2.21	0.40
1:A:331:GLU:OE1	1:A:331:GLU:N	2.55	0.40
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.51	0.40
1:B:508:ARG:NE	2:B:742:HOH:O	2.29	0.40
1:A:366:CYS:O	1:A:367:SER:HB2	2.21	0.40
1:A:544:GLN:O	1:A:546:ASP:N	2.52	0.40
1:B:44:SER:O	1:B:47:LEU:HB2	2.21	0.40
1:B:517:ARG:HH11	1:B:517:ARG:CG	2.34	0.40
1:B:556:SER:C	1:B:558:GLY:N	2.74	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	564/570 (99%)	532 (94%)	23 (4%)	9 (2%)	9 4
1	B	563/570 (99%)	529 (94%)	22 (4%)	12 (2%)	7 2
All	All	1127/1140 (99%)	1061 (94%)	45 (4%)	21 (2%)	8 3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	540	PRO
1	A	542	ALA
1	A	545	LEU
1	B	103	TYR
1	B	540	PRO
1	B	542	ALA
1	B	548	SER
1	B	549	GLY
1	B	556	SER
1	A	23	ILE
1	A	543	SER
1	B	515	GLY
1	B	563	SER
1	B	149	PRO
1	A	380	ARG
1	B	547	LEU
1	A	26	LEU
1	B	151	LYS
1	B	544	GLN
1	A	376	ALA

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	475/485 (98%)	443 (93%)	32 (7%)	16 11
1	B	475/485 (98%)	428 (90%)	47 (10%)	8 4
All	All	950/970 (98%)	871 (92%)	79 (8%)	11 7

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	26	LEU
1	A	28	ASN
1	A	31	LEU
1	A	47	LEU
1	A	52	VAL
1	A	56	ARG
1	A	68	LEU
1	A	77	THR
1	A	126	LEU
1	A	130	THR
1	A	144	VAL
1	A	210	SER
1	A	280	ARG
1	A	287	THR
1	A	309	GLN
1	A	313	MET
1	A	322	VAL
1	A	330	GLN
1	A	331	GLU
1	A	345	ARG
1	A	362	LEU
1	A	384	LEU
1	A	386	ARG
1	A	425	LEU
1	A	433	LEU
1	A	434	LEU
1	A	459	LEU
1	A	508	ARG
1	A	514	GLN
1	A	534	LEU
1	A	547	LEU
1	B	10	LEU
1	B	20	LYS
1	B	24	ASN

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Mol	Chain	Res	Type
1	B	47	LEU
1	B	52	VAL
1	B	56	ARG
1	B	57	LEU
1	B	68	LEU
1	B	77	THR
1	B	82	LEU
1	B	94	PRO
1	B	96	SER
1	B	106	LYS
1	B	126	LEU
1	B	144	VAL
1	B	148	GLN
1	B	149	PRO
1	B	158	ARG
1	B	163	PRO
1	B	180	SER
1	B	221	THR
1	B	222	ARG
1	B	262	ILE
1	B	274	CYS
1	B	277	ARG
1	B	287	THR
1	B	308	LEU
1	B	310	ASP
1	B	313	MET
1	B	330	GLN
1	B	337	ARG
1	B	364	THR
1	B	365	SER
1	B	367	SER
1	B	405	ILE
1	B	425	LEU
1	B	439	LEU
1	B	453	SER
1	B	459	LEU
1	B	465	ARG
1	B	490	ARG
1	B	498	ARG
1	B	517	ARG
1	B	531	ARG
1	B	534	LEU

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Mol	Chain	Res	Type
1	B	538	PRO
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	33	HIS
1	A	34	HIS
1	A	35	ASN
1	A	49	GLN
1	A	206	ASN
1	A	272	GLN
1	A	273	ASN
1	A	309	GLN
1	A	428	HIS
1	A	446	GLN
1	A	483	ASN
1	A	514	GLN
1	B	24	ASN
1	B	34	HIS
1	B	35	ASN
1	B	49	GLN
1	B	148	GLN
1	B	206	ASN
1	B	273	ASN
1	B	316	ASN
1	B	355	GLN
1	B	374	HIS
1	B	483	ASN
1	B	514	GLN

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.