



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 AM UTC

PDB ID : 1WAS / pdb_00001was
Title : THE THREE-DIMENSIONAL STRUCTURE OF THE LIGAND-BINDING
DOMAIN OF A WILD-TYPE BACTERIAL CHEMOTAXIS RECEPTOR
Authors : Kim, S.-H.
Deposited on : 1993-03-09
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

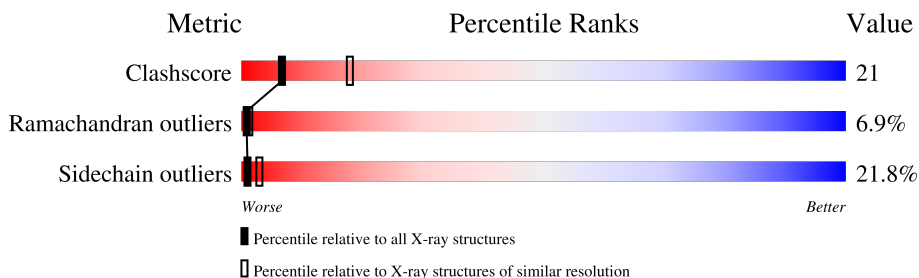
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	146	16% 51% 22% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1144 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 BACTERIAL ASPARTATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1144	703	204	228	9	5	0	0

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. 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: BACTERIAL ASPARTATE RECEPTOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	65.05Å 65.05Å 72.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1144	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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	2.16	33/1160 (2.8%)	2.74	110/1565 (7.0%)

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 (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	ASN	C-N	7.02	1.43	1.33
1	A	152	GLN	N-CA	6.83	1.55	1.45
1	A	118	GLU	N-CA	6.70	1.54	1.46
1	A	100	ALA	C-O	-6.56	1.16	1.24
1	A	150	PHE	CA-CB	6.51	1.61	1.52
1	A	179	THR	CA-C	-6.39	1.45	1.52
1	A	103	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	55	SER	N-CA	-6.20	1.38	1.46
1	A	55	SER	C-O	-6.12	1.16	1.24
1	A	101	ALA	C-O	6.07	1.31	1.24
1	A	159	ASN	CA-CB	-6.06	1.43	1.53
1	A	84	SER	CA-C	6.04	1.60	1.52
1	A	48	GLN	CA-C	-6.02	1.44	1.52
1	A	178	GLN	C-N	5.95	1.41	1.33
1	A	173	GLU	N-CA	-5.90	1.39	1.46
1	A	86	LYS	CA-C	-5.90	1.44	1.52
1	A	172	SER	CA-CB	-5.86	1.44	1.53
1	A	68	SER	C-O	-5.84	1.17	1.24
1	A	136	GLU	C-O	5.84	1.31	1.24
1	A	73	ARG	NE-CZ	5.72	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	HIS	C-N	-5.71	1.26	1.34
1	A	150	PHE	C-N	5.71	1.41	1.33
1	A	42	ILE	CA-CB	5.60	1.61	1.54
1	A	87	THR	CA-C	5.52	1.60	1.52
1	A	96	THR	C-N	5.50	1.41	1.33
1	A	162	GLY	C-O	5.50	1.30	1.23
1	A	136	GLU	CA-CB	-5.46	1.45	1.53
1	A	150	PHE	CA-C	5.46	1.60	1.53
1	A	171	VAL	CA-CB	5.46	1.62	1.54
1	A	61	LEU	CB-CG	5.46	1.64	1.53
1	A	113	LEU	CA-CB	5.36	1.64	1.53
1	A	156	GLY	N-CA	5.34	1.52	1.45
1	A	150	PHE	CB-CG	5.29	1.62	1.50

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PHE	CA-CB-CG	-16.54	97.26	113.80
1	A	58	ASP	CA-CB-CG	12.61	125.21	112.60
1	A	109	ASN	N-CA-C	-11.24	99.91	112.72
1	A	111	THR	N-CA-C	11.03	123.84	109.83
1	A	131	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	A	94	LYS	N-CA-C	-9.70	98.97	112.45
1	A	150	PHE	CA-CB-CG	9.62	123.42	113.80
1	A	152	GLN	N-CA-C	8.82	121.04	109.83
1	A	41	VAL	CA-C-O	-8.60	112.01	120.95
1	A	122	ASN	CB-CG-ND2	8.56	129.24	116.40
1	A	131	GLN	CG-CD-NE2	8.31	128.87	116.40
1	A	86	LYS	N-CA-C	8.29	128.46	110.80
1	A	92	ASN	OD1-CG-ND2	-8.14	114.46	122.60
1	A	61	LEU	N-CA-C	-7.99	99.34	111.56
1	A	43	SER	N-CA-C	7.99	121.08	111.82
1	A	105	ALA	CA-C-O	7.96	129.13	119.97
1	A	159	ASN	CA-CB-CG	-7.94	104.66	112.60
1	A	47	ARG	N-CA-C	-7.93	101.42	112.45
1	A	177	ARG	N-CA-C	-7.73	99.93	110.68
1	A	154	THR	N-CA-C	-7.65	102.94	111.28
1	A	75	MET	N-CA-C	7.59	120.33	110.53
1	A	54	THR	CA-C-O	-7.53	112.49	120.55
1	A	166	GLY	N-CA-C	-7.40	103.91	112.50
1	A	78	ALA	CA-C-N	7.38	130.03	120.44
1	A	78	ALA	C-N-CA	7.38	130.03	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	SER	N-CA-C	-7.37	96.85	108.63
1	A	139	GLN	N-CA-C	-7.21	103.42	111.28
1	A	47	ARG	CA-CB-CG	7.16	128.42	114.10
1	A	62	GLN	OE1-CD-NE2	-7.15	115.45	122.60
1	A	107	PHE	N-CA-C	-7.13	104.44	113.43
1	A	167	ASN	CA-CB-CG	-7.00	105.60	112.60
1	A	119	ALA	N-CA-C	-6.97	95.95	110.80
1	A	161	LEU	CA-C-N	6.95	127.70	119.98
1	A	161	LEU	C-N-CA	6.95	127.70	119.98
1	A	56	THR	CA-C-N	6.90	129.76	120.65
1	A	56	THR	C-N-CA	6.90	129.76	120.65
1	A	111	THR	CA-C-O	6.88	127.68	120.25
1	A	143	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	44	ASN	CA-C-N	6.85	130.14	120.28
1	A	44	ASN	C-N-CA	6.85	130.14	120.28
1	A	73	ARG	O-C-N	-6.80	113.54	122.59
1	A	122	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	A	91	GLN	CA-C-O	6.72	127.88	120.82
1	A	85	ALA	N-CA-C	6.72	125.11	110.80
1	A	96	THR	CB-CA-C	6.68	123.49	110.67
1	A	130	TYR	O-C-N	-6.67	113.32	122.46
1	A	38	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	A	36	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	54	THR	N-CA-C	-6.51	103.45	111.40
1	A	160	ALA	CA-C-O	-6.48	113.68	120.55
1	A	50	GLN	CB-CG-CD	6.48	123.61	112.60
1	A	38	GLN	N-CA-C	6.46	124.56	110.80
1	A	85	ALA	CA-C-O	6.42	129.69	120.51
1	A	84	SER	CA-CB-OG	6.41	123.92	111.10
1	A	49	GLN	CA-C-O	-6.40	114.30	120.90
1	A	54	THR	O-C-N	-6.38	114.45	122.17
1	A	79	SER	O-C-N	6.37	128.63	122.07
1	A	168	TYR	O-C-N	-6.36	114.90	122.15
1	A	141	LEU	N-CA-C	6.34	120.62	113.01
1	A	140	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	89	LEU	N-CA-CB	-6.28	100.63	110.30
1	A	151	ALA	CA-C-N	6.28	129.41	120.49
1	A	151	ALA	C-N-CA	6.28	129.41	120.49
1	A	49	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	A	87	THR	CA-CB-CG2	6.21	121.05	110.50
1	A	62	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	139	GLN	OE1-CD-NE2	-6.16	116.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	LEU	CA-C-N	6.16	126.34	119.32
1	A	113	LEU	C-N-CA	6.16	126.34	119.32
1	A	92	ASN	CB-CG-ND2	6.07	125.50	116.40
1	A	150	PHE	O-C-N	-6.05	113.25	122.08
1	A	88	ASP	O-C-N	-6.04	114.55	122.59
1	A	50	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	128	GLN	OE1-CD-NE2	-6.01	116.58	122.60
1	A	147	ASP	O-C-N	5.94	128.42	122.12
1	A	107	PHE	CA-C-O	-5.93	112.58	119.64
1	A	145	ASN	N-CA-C	5.92	123.40	110.80
1	A	131	GLN	N-CA-C	-5.82	105.01	111.36
1	A	142	ASP	N-CA-C	-5.82	105.28	112.90
1	A	80	ASN	N-CA-C	-5.81	98.42	110.80
1	A	49	GLN	CB-CG-CD	5.81	122.47	112.60
1	A	61	LEU	O-C-N	-5.79	115.66	122.32
1	A	48	GLN	CA-C-O	-5.68	114.82	120.90
1	A	157	MET	CG-SD-CE	-5.67	88.43	100.90
1	A	103	HIS	CA-C-O	-5.62	114.92	120.82
1	A	82	GLN	CA-C-O	5.61	128.01	120.89
1	A	136	GLU	CA-CB-CG	-5.60	102.91	114.10
1	A	148	ALA	CA-C-O	-5.60	113.31	120.31
1	A	120	SER	O-C-N	5.52	127.76	122.07
1	A	134	LEU	CD1-CG-CD2	-5.49	98.72	110.80
1	A	180	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	52	GLU	N-CA-C	-5.43	106.43	113.16
1	A	36	ASN	CA-C-O	5.41	128.25	120.51
1	A	109	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	177	ARG	CA-CB-CG	-5.38	103.35	114.10
1	A	149	TYR	O-C-N	-5.37	115.45	122.59
1	A	43	SER	CA-C-O	5.36	126.13	119.97
1	A	138	ILE	CB-CG1-CD1	5.33	124.99	113.80
1	A	46	LEU	N-CA-CB	5.32	118.52	110.28
1	A	173	GLU	N-CA-C	-5.31	105.39	111.07
1	A	175	LEU	N-CA-C	-5.23	105.25	111.69
1	A	74	MET	CB-CA-C	-5.23	104.58	111.74
1	A	44	ASN	N-CA-C	-5.18	105.70	112.23
1	A	141	LEU	O-C-N	-5.14	115.36	122.46
1	A	178	GLN	CA-CB-CG	5.09	124.28	114.10
1	A	100	ALA	CA-C-N	5.08	127.09	120.28
1	A	100	ALA	C-N-CA	5.08	127.09	120.28
1	A	100	ALA	O-C-N	5.06	127.50	122.08
1	A	140	PHE	O-C-N	-5.05	115.87	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	41	VAL	O-C-N	5.01	126.73	121.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	LEU	Peptide

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	1144	0	1103	48	0
All	All	1144	0	1103	48	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 21.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:HE3	1:A:84:SER:HA	1.64	0.79
1:A:69:ARG:O	1:A:73:ARG:HB2	1.90	0.71
1:A:130:TYR:HD2	1:A:161:LEU:HD12	1.59	0.67
1:A:130:TYR:CD2	1:A:161:LEU:HD12	2.32	0.65
1:A:44:ASN:O	1:A:47:ARG:HG3	1.97	0.64
1:A:62:GLN:HA	1:A:65:ILE:HD12	1.80	0.63
1:A:69:ARG:HB3	1:A:89:LEU:HD23	1.82	0.62
1:A:92:ASN:O	1:A:96:THR:HB	2.03	0.58
1:A:86:LYS:O	1:A:88:ASP:N	2.38	0.57
1:A:170:ARG:HG3	1:A:171:VAL:HG23	1.85	0.57
1:A:95:THR:O	1:A:99:GLN:HG3	2.06	0.55
1:A:74:MET:HE2	1:A:146:MET:HE1	1.90	0.54
1:A:53:LEU:HD21	1:A:123:VAL:HG11	1.90	0.54
1:A:126:LYS:HG3	1:A:164:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:O	1:A:116:MET:HG2	2.11	0.51
1:A:139:GLN:O	1:A:143:ASN:HB2	2.11	0.51
1:A:70:SER:O	1:A:74:MET:SD	2.69	0.50
1:A:74:MET:HE2	1:A:146:MET:CE	2.41	0.50
1:A:86:LYS:HA	1:A:90:LEU:HB2	1.93	0.50
1:A:141:LEU:HD13	1:A:149:TYR:CD2	2.47	0.50
1:A:116:MET:HE3	1:A:175:LEU:HD12	1.94	0.50
1:A:96:THR:HA	1:A:99:GLN:HE21	1.76	0.50
1:A:126:LYS:O	1:A:129:ARG:HG2	2.12	0.49
1:A:126:LYS:HG3	1:A:164:ALA:CB	2.43	0.48
1:A:140:PHE:CD2	1:A:149:TYR:HA	2.50	0.47
1:A:119:ALA:HB1	1:A:168:TYR:HD1	1.79	0.47
1:A:137:LEU:N	1:A:137:LEU:HD23	2.30	0.46
1:A:90:LEU:HD11	1:A:142:ASP:HB3	1.97	0.46
1:A:67:LEU:HD13	1:A:137:LEU:HD12	1.97	0.45
1:A:66:ASN:HB2	1:A:93:ALA:HB2	1.98	0.45
1:A:56:THR:O	1:A:60:MET:HG3	2.17	0.45
1:A:170:ARG:HG3	1:A:171:VAL:N	2.31	0.44
1:A:51:SER:O	1:A:54:THR:HB	2.17	0.44
1:A:88:ASP:HB3	1:A:89:LEU:HD12	1.99	0.44
1:A:137:LEU:HD21	1:A:152:GLN:CD	2.43	0.43
1:A:79:SER:O	1:A:81:GLN:N	2.52	0.43
1:A:119:ALA:HB1	1:A:168:TYR:CD1	2.54	0.43
1:A:137:LEU:HD21	1:A:152:GLN:NE2	2.34	0.43
1:A:70:SER:O	1:A:71:ALA:C	2.60	0.43
1:A:52:GLU:HA	1:A:55:SER:OG	2.19	0.42
1:A:102:ALA:O	1:A:106:ASN:ND2	2.51	0.42
1:A:173:GLU:O	1:A:176:TYR:N	2.52	0.42
1:A:88:ASP:O	1:A:91:GLN:HG3	2.21	0.41
1:A:59:LEU:HD11	1:A:99:GLN:NE2	2.36	0.41
1:A:64:ARG:NH1	1:A:158:GLN:OE1	2.54	0.40
1:A:173:GLU:O	1:A:177:ARG:N	2.54	0.40
1:A:90:LEU:CD1	1:A:142:ASP:HB3	2.51	0.40
1:A:113:LEU:O	1:A:115:ALA:N	2.54	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	144/146 (99%)	108 (75%)	26 (18%)	10 (7%)	1 1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	85	ALA
1	A	87	THR
1	A	78	ALA
1	A	145	ASN
1	A	37	GLN
1	A	178	GLN
1	A	40	PHE
1	A	86	LYS
1	A	144	GLY

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	119/119 (100%)	93 (78%)	26 (22%)	1 3

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	42	ILE
1	A	45	GLU
1	A	46	LEU
1	A	47	ARG
1	A	61	LEU
1	A	62	GLN
1	A	64	ARG
1	A	66	ASN
1	A	73	ARG
1	A	74	MET
1	A	76	MET
1	A	84	SER
1	A	86	LYS
1	A	87	THR
1	A	96	THR
1	A	108	LYS
1	A	126	LYS
1	A	134	LEU
1	A	139	GLN
1	A	141	LEU
1	A	145	ASN
1	A	155	GLN
1	A	161	LEU
1	A	165	LEU
1	A	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	62	GLN
1	A	81	GLN
1	A	99	GLN
1	A	109	ASN
1	A	145	ASN
1	A	152	GLN
1	A	167	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.