



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:28 PM UTC

PDB ID : 2DP4 / pdb_00002dp4
Title : Crystal structure of the complex formed between proteinase K and a human lactoferrin fragment at 2.9 Å resolution
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on : 2006-05-05
Resolution : 2.90 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

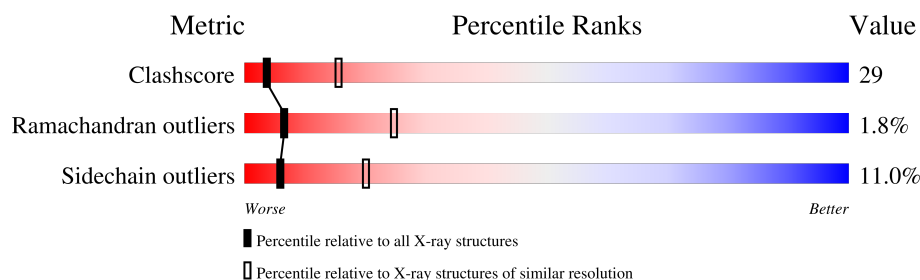
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	E	279	
2	I	8	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2201 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 Proteinase K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	279	Total	C	N	O	S	0	0	0
			2029	1247	357	415	10			

- Molecule 2 is a protein called 8-mer peptide from Lactotransferrin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	0	0	0
			60	33	11	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	107	Total	O	0	0
			107	107		
3	I	5	Total	O	0	0
			5	5		

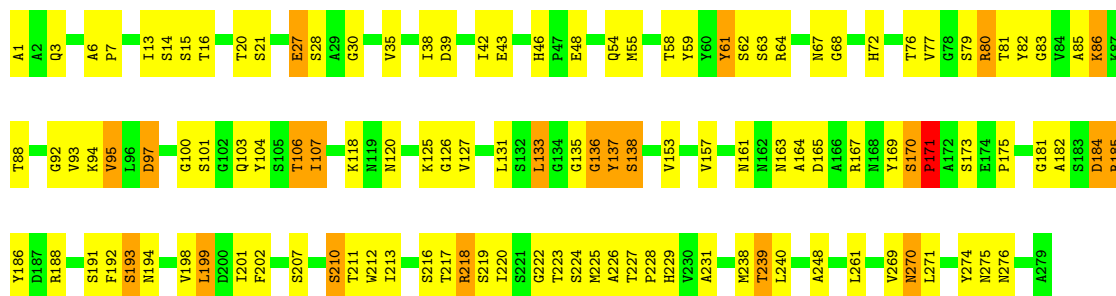
3 Residue-property plots

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: Proteinase K

Chain E: 



• Molecule 2: 8-mer peptide from Lactotransferrin

Chain I: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.40 Å 68.40 Å 108.13 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.80 – 2.90	Depositor
% Data completeness (in resolution range)	92.8 (11.80-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.193 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2201	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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	E	0.71	2/2068 (0.1%)	1.62	24/2810 (0.9%)
2	I	1.61	0/59	4.29	17/76 (22.4%)
All	All	0.75	2/2127 (0.1%)	1.74	41/2886 (1.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	210	SER	C-O	5.82	1.30	1.23
1	E	171	PRO	CA-CB	-5.24	1.46	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	SER	CA-C-N	39.94	169.76	119.84
1	E	170	SER	C-N-CA	39.94	169.76	119.84
1	E	170	SER	C-N-CD	-13.81	68.37	125.00
2	I	3	GLU	N-CA-C	13.74	126.34	108.34
2	I	6	GLU	N-CA-C	-12.12	97.76	112.54
2	I	4	GLN	OE1-CD-NE2	-10.71	111.89	122.60
1	E	136	GLY	CA-C-N	9.98	140.61	121.54
1	E	136	GLY	C-N-CA	9.98	140.61	121.54
2	I	2	ASP	CA-C-N	-9.89	106.17	122.39
2	I	2	ASP	C-N-CA	-9.89	106.17	122.39
2	I	2	ASP	CA-CB-CG	9.37	121.97	112.60
2	I	4	GLN	N-CA-C	7.71	127.23	110.80
1	E	107	ILE	N-CA-C	-7.18	103.30	110.62
1	E	81	THR	N-CA-CB	-7.14	99.92	110.49
1	E	171	PRO	CA-N-CD	-7.02	102.17	112.00
1	E	248	ALA	N-CA-C	6.75	119.25	111.02
2	I	4	GLN	CB-CG-CD	-6.73	101.16	112.60
1	E	275	ASN	N-CA-C	6.66	121.02	113.02
1	E	137	TYR	N-CA-CB	6.25	121.05	110.49
2	I	4	GLN	CG-CD-NE2	6.17	125.66	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	185	ARG	N-CA-C	6.15	123.90	110.80
2	I	7	ASN	O-C-N	6.02	130.59	122.59
1	E	231	ALA	N-CA-C	-6.01	104.64	111.14
2	I	5	GLY	CA-C-N	-5.77	111.09	120.72
2	I	5	GLY	C-N-CA	-5.77	111.09	120.72
1	E	80	ARG	N-CA-C	5.53	120.50	111.37
1	E	14	SER	N-CA-C	-5.46	106.50	112.72
1	E	223	THR	N-CA-C	-5.43	106.73	113.19
2	I	5	GLY	N-CA-C	-5.36	100.47	113.18
1	E	107	ILE	CB-CA-C	-5.31	104.97	112.14
2	I	3	GLU	CA-C-N	5.25	131.57	121.54
2	I	3	GLU	C-N-CA	5.25	131.57	121.54
1	E	193	SER	N-CA-C	5.19	117.74	109.96
1	E	86	LYS	N-CA-C	5.18	119.09	112.87
1	E	43	GLU	N-CA-C	-5.18	98.24	107.98
1	E	95	VAL	N-CA-C	-5.09	107.46	113.42
1	E	171	PRO	CA-C-N	5.02	126.97	120.44
1	E	171	PRO	C-N-CA	5.02	126.97	120.44
2	I	1	GLY	CA-C-N	5.02	131.13	121.54
2	I	1	GLY	C-N-CA	5.02	131.13	121.54
1	E	97	ASP	N-CA-CB	-5.01	102.99	110.60

There are no chirality outliers.

There are no planarity outliers.

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	E	2029	0	1935	115	0
2	I	60	0	51	20	0
3	E	107	0	0	8	0
3	I	5	0	0	3	0
All	All	2201	0	1986	118	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 29.

All (118) 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:E:30:GLY:HA2	1:E:239:THR:HG21	1.52	0.89
1:E:224:SER:OG	2:I:2:ASP:HB3	1.74	0.88
1:E:58:THR:HG21	1:E:62:SER:O	1.77	0.84
1:E:212:TRP:CD2	1:E:218:ARG:HD3	2.12	0.84
1:E:261:LEU:H	1:E:270:ASN:HD21	1.27	0.83
1:E:185:ARG:HD2	3:E:354:HOH:O	1.86	0.75
1:E:218:ARG:NH2	2:I:6:GLU:HB2	2.03	0.74
1:E:46:HIS:HD2	1:E:48:GLU:H	1.34	0.73
1:E:35:VAL:HG11	1:E:77:VAL:HG11	1.71	0.72
1:E:64:ARG:HD3	3:E:358:HOH:O	1.92	0.69
1:E:220:ILE:HB	2:I:4:GLN:O	1.92	0.68
1:E:100:GLY:HA3	2:I:8:LYS:C	2.17	0.68
1:E:207:SER:HB3	3:E:306:HOH:O	1.95	0.67
1:E:133:LEU:C	1:E:133:LEU:HD22	2.21	0.66
1:E:97:ASP:HB3	1:E:101:SER:O	1.95	0.66
1:E:64:ARG:HH11	1:E:64:ARG:HG3	1.61	0.65
1:E:30:GLY:HA2	1:E:239:THR:CG2	2.27	0.65
1:E:42:ILE:HD12	1:E:92:GLY:HA3	1.81	0.63
1:E:126:GLY:HA3	1:E:238:MET:HE3	1.82	0.62
1:E:68:GLY:HA2	1:E:213:ILE:HG23	1.83	0.61
1:E:185:ARG:CD	3:E:354:HOH:O	2.45	0.60
1:E:173:SER:HA	1:E:198:VAL:HG21	1.83	0.60
1:E:125:LYS:CG	1:E:239:THR:HA	2.32	0.60
1:E:135:GLY:O	1:E:169:TYR:HD1	1.84	0.60
1:E:38:ILE:HB	1:E:131:LEU:HD23	1.82	0.60
1:E:163:ASN:ND2	1:E:191:SER:O	2.36	0.59
1:E:38:ILE:HG22	1:E:95:VAL:HG21	1.84	0.59
1:E:220:ILE:HD11	1:E:225:MET:HE2	1.84	0.59
1:E:269:VAL:HB	1:E:271:LEU:HD12	1.86	0.58
1:E:220:ILE:CG2	2:I:5:GLY:HA2	2.33	0.58
1:E:30:GLY:CA	1:E:239:THR:HG21	2.31	0.57
1:E:72:HIS:NE2	1:E:210:SER:HB3	2.20	0.57
1:E:58:THR:HG23	1:E:94:LYS:HB3	1.87	0.57
1:E:184:ASP:C	1:E:184:ASP:OD1	2.48	0.57
1:E:165:ASP:OD1	1:E:167:ARG:HD2	2.05	0.56
2:I:3:GLU:CD	3:I:40:HOH:O	2.47	0.56
1:E:165:ASP:CG	1:E:167:ARG:HD2	2.32	0.55
1:E:186:TYR:HD2	1:E:188:ARG:NH2	2.05	0.55
1:E:46:HIS:CD2	1:E:48:GLU:H	2.20	0.55
1:E:225:MET:SD	1:E:225:MET:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:PHE:CE1	1:E:222:GLY:HA2	2.43	0.54
1:E:72:HIS:CD2	1:E:210:SER:HB3	2.43	0.54
1:E:61:TYR:CD1	1:E:61:TYR:N	2.67	0.54
1:E:79:SER:H	1:E:83:GLY:HA3	1.72	0.54
1:E:201:ILE:HG13	1:E:202:PHE:N	2.22	0.53
1:E:82:TYR:CD2	1:E:211:THR:CG2	2.92	0.53
1:E:131:LEU:HD22	1:E:133:LEU:HD11	1.91	0.53
1:E:227:THR:N	1:E:228:PRO:HD2	2.25	0.52
1:E:42:ILE:HD12	1:E:92:GLY:CA	2.40	0.52
2:I:3:GLU:HG2	3:I:40:HOH:O	2.09	0.52
1:E:93:VAL:HG12	1:E:95:VAL:HG13	1.92	0.52
1:E:72:HIS:CE1	1:E:210:SER:HB3	2.46	0.51
1:E:3:GLN:HE22	1:E:86:LYS:NZ	2.09	0.51
1:E:76:THR:O	1:E:83:GLY:HA2	2.11	0.50
1:E:213:ILE:C	1:E:213:ILE:HD12	2.35	0.50
1:E:100:GLY:CA	2:I:8:LYS:C	2.83	0.50
1:E:125:LYS:HG2	1:E:239:THR:HA	1.94	0.50
1:E:125:LYS:HG2	1:E:239:THR:HB	1.92	0.50
1:E:133:LEU:C	1:E:133:LEU:CD2	2.85	0.50
1:E:137:TYR:O	1:E:138:SER:HB2	2.11	0.50
1:E:222:GLY:C	1:E:224:SER:H	2.20	0.49
1:E:58:THR:HG22	1:E:59:TYR:H	1.77	0.49
1:E:136:GLY:HA2	1:E:169:TYR:HA	1.95	0.49
1:E:220:ILE:HG22	2:I:5:GLY:HA2	1.95	0.49
1:E:64:ARG:HG3	1:E:64:ARG:NH1	2.26	0.49
1:E:133:LEU:HA	2:I:1:GLY:N	2.28	0.49
1:E:137:TYR:CG	1:E:138:SER:N	2.81	0.48
1:E:212:TRP:CG	1:E:218:ARG:HD3	2.47	0.48
1:E:103:GLN:HB2	1:E:106:THR:HG23	1.95	0.48
1:E:226:ALA:O	1:E:229:HIS:HB2	2.14	0.48
1:E:126:GLY:HA3	1:E:238:MET:CE	2.44	0.48
1:E:131:LEU:HB2	1:E:157:VAL:HG12	1.95	0.48
1:E:169:TYR:HB3	3:E:298:HOH:O	2.14	0.47
1:E:133:LEU:HA	2:I:1:GLY:H2	1.78	0.47
1:E:182:ALA:HB3	1:E:193:SER:HB2	1.95	0.47
1:E:85:ALA:O	1:E:88:THR:HG22	2.15	0.47
1:E:224:SER:OG	2:I:2:ASP:CB	2.57	0.46
1:E:58:THR:HG23	1:E:94:LYS:HD3	1.96	0.46
1:E:220:ILE:HG21	2:I:5:GLY:HA2	1.98	0.45
1:E:27:GLU:CD	1:E:27:GLU:H	2.23	0.45
1:E:164:ALA:H	1:E:194:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:HG21	2:I:5:GLY:CA	2.47	0.45
1:E:1:ALA:HB2	1:E:27:GLU:OE1	2.16	0.44
1:E:104:TYR:OH	1:E:135:GLY:HA3	2.16	0.44
1:E:100:GLY:HA3	2:I:8:LYS:HG2	2.00	0.44
1:E:212:TRP:N	1:E:216:SER:O	2.36	0.44
1:E:133:LEU:HD22	1:E:133:LEU:O	2.17	0.44
1:E:15:SER:HB2	3:E:366:HOH:O	2.17	0.44
1:E:38:ILE:HG22	1:E:95:VAL:CG2	2.46	0.43
1:E:82:TYR:CD2	1:E:211:THR:HG23	2.53	0.43
1:E:82:TYR:HD2	1:E:211:THR:CG2	2.31	0.43
1:E:222:GLY:C	1:E:224:SER:N	2.74	0.43
1:E:202:PHE:HB2	1:E:271:LEU:O	2.19	0.43
1:E:240:LEU:HD12	1:E:240:LEU:HA	1.80	0.43
1:E:270:ASN:ND2	3:E:317:HOH:O	2.52	0.43
1:E:55:MET:HE2	1:E:63:SER:O	2.18	0.43
1:E:217:THR:O	1:E:218:ARG:HB3	2.18	0.43
1:E:54:GLN:HG2	1:E:55:MET:O	2.19	0.43
1:E:6:ALA:HB1	1:E:7:PRO:CD	2.49	0.42
1:E:173:SER:O	1:E:175:PRO:HD3	2.19	0.42
1:E:13:ILE:O	1:E:274:TYR:HD1	2.03	0.42
1:E:3:GLN:HE22	1:E:86:LYS:HZ1	1.66	0.42
2:I:3:GLU:CG	3:I:40:HOH:O	2.67	0.42
1:E:201:ILE:HG13	1:E:202:PHE:H	1.83	0.42
1:E:127:VAL:HG12	1:E:153:VAL:HG13	2.01	0.42
1:E:100:GLY:HA2	2:I:8:LYS:O	2.19	0.42
1:E:3:GLN:NE2	1:E:86:LYS:NZ	2.69	0.41
1:E:125:LYS:HG2	1:E:239:THR:CB	2.51	0.41
1:E:210:SER:O	1:E:217:THR:HB	2.21	0.41
1:E:186:TYR:CD2	1:E:188:ARG:NH2	2.86	0.41
1:E:103:GLN:O	1:E:107:ILE:HG12	2.21	0.41
1:E:67:ASN:ND2	2:I:8:LYS:O	2.54	0.41
1:E:80:ARG:NH2	3:E:367:HOH:O	2.41	0.41
1:E:20:THR:HG22	1:E:21:SER:N	2.36	0.40
1:E:181:GLY:HA3	1:E:199:LEU:HD21	2.03	0.40
1:E:218:ARG:HH22	2:I:6:GLU:HB2	1.82	0.40
1:E:161:ASN:HA	1:E:192:PHE:O	2.21	0.40
1:E:161:ASN:ND2	2:I:2:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	277/279 (99%)	256 (92%)	19 (7%)	2 (1%)	18	48
2	I	6/8 (75%)	2 (33%)	1 (17%)	3 (50%)	0	0
All	All	283/287 (99%)	258 (91%)	20 (7%)	5 (2%)	6	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	138	SER
1	E	171	PRO
2	I	2	ASP
2	I	4	GLN
2	I	7	ASN

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	E	213/213 (100%)	195 (92%)	18 (8%)	10	31
2	I	6/6 (100%)	0	6 (100%)	0	0
All	All	219/219 (100%)	195 (89%)	24 (11%)	6	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	16	THR

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Mol	Chain	Res	Type
1	E	27	GLU
1	E	28	SER
1	E	39	ASP
1	E	61	TYR
1	E	106	THR
1	E	118	LYS
1	E	120	ASN
1	E	133	LEU
1	E	170	SER
1	E	171	PRO
1	E	184	ASP
1	E	199	LEU
1	E	218	ARG
1	E	219	SER
1	E	239	THR
1	E	270	ASN
1	E	276	ASN
2	I	2	ASP
2	I	3	GLU
2	I	4	GLN
2	I	6	GLU
2	I	7	ASN
2	I	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	GLN
1	E	5	ASN
1	E	31	GLN
1	E	46	HIS
1	E	54	GLN
1	E	67	ASN
1	E	119	ASN
1	E	168	ASN
1	E	194	ASN
1	E	257	ASN
1	E	270	ASN
2	I	4	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 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.