



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:25 PM UTC

PDB ID : 1X10 / pdb_00001x10
Title : Structure of Mutant Pyrrolidone Carboxyl Peptidase (E192A) from a Hyper-thermophile, *Pyrococcus furiosus*
Authors : Kaushik, J.K.; Yamagata, Y.; Ogasahara, K.; Yutani, K.
Deposited on : 2005-03-31
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 ⓘ 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

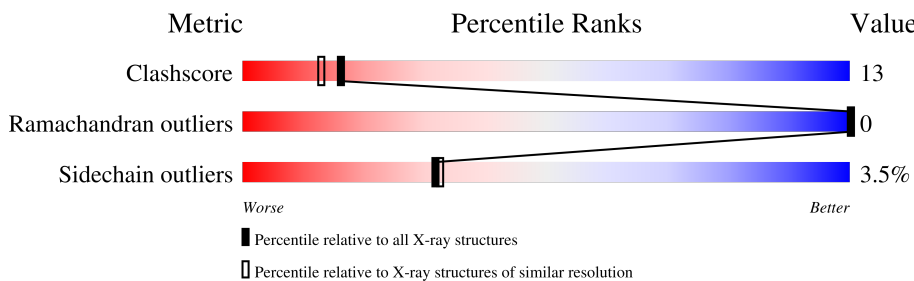
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	208	73% 25% .
1	B	208	73% 25% .
1	C	208	73% 25% .
1	D	208	73% 25% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7128 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 Pyrrolidone-carboxylate peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1601	1038	263	294	6			
1	B	208	Total	C	N	O	S	0	0	0
			1601	1038	263	294	6			
1	C	208	Total	C	N	O	S	0	0	0
			1601	1038	263	294	6			
1	D	208	Total	C	N	O	S	0	0	0
			1601	1038	263	294	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	CYS	engineered mutation	UNP O73944
A	188	SER	CYS	engineered mutation	UNP O73944
A	192	ALA	GLU	engineered mutation	UNP O73944
B	142	SER	CYS	engineered mutation	UNP O73944
B	188	SER	CYS	engineered mutation	UNP O73944
B	192	ALA	GLU	engineered mutation	UNP O73944
C	142	SER	CYS	engineered mutation	UNP O73944
C	188	SER	CYS	engineered mutation	UNP O73944
C	192	ALA	GLU	engineered mutation	UNP O73944
D	142	SER	CYS	engineered mutation	UNP O73944
D	188	SER	CYS	engineered mutation	UNP O73944
D	192	ALA	GLU	engineered mutation	UNP O73944

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	183	Total	O	0	0
			183	183		
2	B	192	Total	O	0	0
			192	192		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	169	Total 169	O 169	0	0
2	D	180	Total 180	O 180	0	0



4 Data and refinement statistics

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	47.44 Å 103.96 Å 187.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.4 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7128	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	0.36	0/1635	0.88	4/2211 (0.2%)
1	B	0.36	0/1635	0.87	4/2211 (0.2%)
1	C	0.35	0/1635	0.88	4/2211 (0.2%)
1	D	0.36	0/1635	0.87	4/2211 (0.2%)
All	All	0.36	0/6540	0.87	16/8844 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ILE	N-CA-C	7.05	117.81	110.62
1	C	117	ILE	N-CA-C	6.66	117.41	110.62
1	B	117	ILE	N-CA-C	6.66	117.41	110.62
1	A	117	ILE	N-CA-C	6.12	117.59	110.62
1	D	81	ILE	N-CA-C	5.91	117.19	108.45
1	A	81	ILE	N-CA-C	5.80	117.04	108.45
1	B	81	ILE	N-CA-C	5.67	116.83	108.45
1	C	81	ILE	N-CA-C	5.59	116.72	108.45
1	D	141	LEU	N-CA-C	5.34	118.02	111.82
1	C	141	LEU	N-CA-C	5.23	117.89	111.82
1	B	141	LEU	N-CA-C	5.18	117.83	111.82
1	D	62	ASP	N-CA-C	-5.15	106.16	112.90
1	A	141	LEU	N-CA-C	5.07	117.69	111.82
1	B	103	ILE	N-CA-C	-5.06	105.91	110.82
1	C	62	ASP	N-CA-C	-5.06	106.27	112.90
1	A	62	ASP	N-CA-C	-5.05	106.29	112.90

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	A	1601	0	1670	45	0
1	B	1601	0	1670	47	1
1	C	1601	0	1670	45	0
1	D	1601	0	1670	46	1
2	A	183	0	0	6	0
2	B	192	0	0	4	0
2	C	169	0	0	8	0
2	D	180	0	0	6	0
All	All	7128	0	6680	171	1

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 (171) 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:1:MET:HE1	1:B:207:LEU:HD12	1.52	0.92
1:C:1:MET:HE1	1:C:207:LEU:HD12	1.52	0.92
1:D:1:MET:HE1	1:D:207:LEU:HD12	1.54	0.90
1:A:1:MET:HE1	1:A:207:LEU:HD12	1.53	0.89
1:D:208:LEU:HB3	2:D:209:HOH:O	1.85	0.77
1:C:99:GLU:HG2	2:C:282:HOH:O	1.84	0.76
1:D:21:ARG:HG3	2:D:345:HOH:O	1.86	0.75
1:A:121:MET:SD	1:A:133:ILE:HD13	2.31	0.71
1:D:121:MET:SD	1:D:133:ILE:HD13	2.31	0.71
1:A:181:GLY:HA2	1:B:89:ARG:NH1	2.06	0.70
1:C:121:MET:SD	1:C:133:ILE:HD13	2.33	0.69
1:B:121:MET:SD	1:B:133:ILE:HD13	2.33	0.68
1:B:100:ASP:HA	2:B:364:HOH:O	1.93	0.68
1:D:70:ALA:HB1	1:D:73:ARG:HD3	1.76	0.67
1:A:70:ALA:HB1	1:A:73:ARG:HD3	1.76	0.67
1:C:70:ALA:HB1	1:C:73:ARG:HD3	1.77	0.67
1:A:21:ARG:HG3	2:A:329:HOH:O	1.95	0.67
1:A:160:LYS:HG3	2:A:295:HOH:O	1.95	0.66
1:A:123:LYS:HE2	1:A:127:ARG:NH1	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LYS:HE2	1:D:127:ARG:NH1	2.12	0.65
1:B:70:ALA:HB1	1:B:73:ARG:HD3	1.78	0.65
1:B:123:LYS:HE2	1:B:127:ARG:NH1	2.13	0.63
1:A:83:VAL:HG21	1:A:139:LEU:HD21	1.81	0.63
1:C:1:MET:HB2	2:C:343:HOH:O	1.98	0.63
1:C:123:LYS:HE2	1:C:127:ARG:NH1	2.13	0.62
1:D:83:VAL:HG21	1:D:139:LEU:HD21	1.82	0.62
1:C:122:LYS:HD2	1:C:122:LYS:C	2.25	0.61
1:B:83:VAL:HG21	1:B:139:LEU:HD21	1.82	0.61
1:C:83:VAL:HG21	1:C:139:LEU:HD21	1.83	0.61
1:C:160:LYS:HG3	2:C:266:HOH:O	2.01	0.61
1:C:174:ILE:HD12	1:C:184:PRO:HG2	1.82	0.60
1:A:122:LYS:HD2	1:A:122:LYS:C	2.26	0.60
1:B:174:ILE:HD12	1:B:184:PRO:HG2	1.84	0.59
1:A:99:GLU:HG2	2:A:250:HOH:O	2.02	0.59
1:A:174:ILE:HD12	1:A:184:PRO:HG2	1.84	0.59
1:B:122:LYS:HD2	1:B:122:LYS:C	2.29	0.58
1:D:122:LYS:HD2	1:D:122:LYS:C	2.28	0.58
1:D:174:ILE:HD12	1:D:184:PRO:HG2	1.84	0.58
1:C:122:LYS:HD3	1:C:126:GLU:OE1	2.04	0.58
1:A:122:LYS:HD3	1:A:126:GLU:OE1	2.04	0.57
1:B:122:LYS:HD3	1:B:126:GLU:OE1	2.05	0.57
1:D:80:ARG:HD2	1:D:135:ASN:ND2	2.20	0.57
1:C:80:ARG:HD2	1:C:135:ASN:ND2	2.20	0.57
1:A:15:LYS:HD2	1:A:15:LYS:N	2.20	0.57
1:B:80:ARG:HD2	1:B:135:ASN:ND2	2.19	0.57
1:D:122:LYS:HD3	1:D:126:GLU:OE1	2.05	0.57
1:D:122:LYS:HE3	2:D:354:HOH:O	2.04	0.56
1:B:73:ARG:HD2	2:B:261:HOH:O	2.05	0.56
1:C:73:ARG:HD2	2:C:223:HOH:O	2.06	0.56
1:A:80:ARG:HD2	1:A:135:ASN:ND2	2.21	0.55
1:A:96:LYS:HE2	2:A:353:HOH:O	2.05	0.55
1:C:49:LYS:O	1:C:53:GLU:HG2	2.06	0.55
1:B:15:LYS:N	1:B:15:LYS:HD2	2.21	0.54
1:A:49:LYS:O	1:A:53:GLU:HG2	2.07	0.54
1:A:208:LEU:HB3	2:A:304:HOH:O	2.07	0.54
1:C:1:MET:HE3	1:C:204:LEU:HD23	1.88	0.54
1:D:15:LYS:N	1:D:15:LYS:HD2	2.21	0.54
1:D:49:LYS:O	1:D:53:GLU:HG2	2.07	0.54
1:A:1:MET:HE1	1:A:207:LEU:CD1	2.34	0.54
1:C:15:LYS:N	1:C:15:LYS:HD2	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LYS:O	1:B:53:GLU:HG2	2.08	0.54
1:B:1:MET:HE3	1:B:204:LEU:HD23	1.90	0.53
1:C:62:ASP:HA	2:C:266:HOH:O	2.07	0.53
1:C:1:MET:HE1	1:C:207:LEU:CD1	2.33	0.53
1:D:1:MET:HE3	1:D:204:LEU:HD23	1.91	0.53
1:D:14:GLU:OE2	1:D:177:LYS:NZ	2.41	0.53
1:B:1:MET:HE1	1:B:207:LEU:CD1	2.33	0.52
1:A:1:MET:HE3	1:A:204:LEU:HD23	1.89	0.52
1:B:182:GLN:HG3	1:B:183:VAL:N	2.25	0.52
1:A:87:ASP:OD1	1:D:80:ARG:NH2	2.35	0.51
1:C:14:GLU:OE2	1:C:177:LYS:NZ	2.41	0.51
1:B:131:ALA:O	1:D:178:ILE:HD13	2.11	0.51
1:D:5:VAL:HG21	1:D:200:ILE:HD11	1.93	0.51
1:A:14:GLU:OE2	1:A:177:LYS:NZ	2.41	0.50
1:D:1:MET:HE1	1:D:207:LEU:CD1	2.35	0.50
1:C:182:GLN:HG3	1:C:183:VAL:N	2.27	0.50
1:C:88:ALA:HB1	1:C:90:ILE:O	2.12	0.49
1:D:182:GLN:HG3	1:D:183:VAL:N	2.26	0.49
1:A:130:PRO:HG2	1:A:187:MET:CE	2.43	0.49
1:D:30:LYS:NZ	1:D:30:LYS:HB3	2.28	0.49
1:D:88:ALA:HB1	1:D:90:ILE:O	2.13	0.49
1:B:30:LYS:HB3	1:B:30:LYS:NZ	2.27	0.49
1:C:1:MET:HE3	1:C:204:LEU:CD2	2.42	0.49
1:C:181:GLY:HA2	1:D:89:ARG:NH1	2.27	0.49
1:C:130:PRO:HG2	1:C:187:MET:CE	2.43	0.49
1:A:1:MET:HE3	1:A:204:LEU:CD2	2.43	0.49
1:B:130:PRO:HG2	1:B:187:MET:CE	2.43	0.48
1:A:182:GLN:HG3	1:A:183:VAL:N	2.27	0.48
1:A:30:LYS:NZ	1:A:30:LYS:HB3	2.28	0.48
1:B:109:THR:HG23	1:C:112:PHE:CE1	2.48	0.48
1:D:83:VAL:HG21	1:D:139:LEU:CD2	2.44	0.48
1:A:88:ALA:HB1	1:A:90:ILE:O	2.14	0.47
1:B:83:VAL:HG21	1:B:139:LEU:CD2	2.44	0.47
1:D:1:MET:HE3	1:D:204:LEU:CD2	2.44	0.47
1:B:5:VAL:HG21	1:B:200:ILE:HD11	1.94	0.47
1:C:5:VAL:HG21	1:C:200:ILE:HD11	1.96	0.47
1:A:76:ILE:O	1:A:131:ALA:HA	2.15	0.47
1:B:49:LYS:HG3	1:B:148:LEU:HD13	1.97	0.47
1:A:5:VAL:HG21	1:A:200:ILE:HD11	1.97	0.47
1:A:73:ARG:O	1:A:168:PRO:HB3	2.15	0.47
1:B:50:GLU:O	1:B:54:LYS:HG3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ILE:O	1:C:131:ALA:HA	2.14	0.47
1:A:49:LYS:HG3	1:A:148:LEU:HD13	1.97	0.47
1:A:83:VAL:HG21	1:A:139:LEU:CD2	2.44	0.47
1:C:30:LYS:NZ	1:C:30:LYS:HB3	2.30	0.47
1:B:1:MET:HE3	1:B:204:LEU:CD2	2.45	0.47
1:C:83:VAL:HG21	1:C:139:LEU:CD2	2.45	0.47
1:D:130:PRO:HG2	1:D:187:MET:CE	2.44	0.47
1:B:122:LYS:HE3	2:B:255:HOH:O	2.14	0.46
1:D:76:ILE:O	1:D:131:ALA:HA	2.15	0.46
1:A:60:LYS:N	1:A:61:PRO:HD3	2.30	0.46
1:C:50:GLU:O	1:C:54:LYS:HG3	2.16	0.46
1:C:49:LYS:HG3	1:C:148:LEU:HD13	1.98	0.46
1:B:76:ILE:O	1:B:131:ALA:HA	2.15	0.46
1:B:88:ALA:HB1	1:B:90:ILE:O	2.14	0.46
1:B:92:ASP:OD1	1:B:96:LYS:NZ	2.49	0.46
1:A:50:GLU:O	1:A:54:LYS:HG3	2.16	0.46
1:C:73:ARG:O	1:C:168:PRO:HB3	2.16	0.46
1:C:181:GLY:HA2	1:D:89:ARG:CZ	2.46	0.46
1:D:73:ARG:O	1:D:168:PRO:HB3	2.16	0.46
1:A:54:LYS:HG3	2:A:361:HOH:O	2.16	0.46
1:B:73:ARG:O	1:B:168:PRO:HB3	2.17	0.45
1:B:60:LYS:N	1:B:61:PRO:HD3	2.31	0.45
1:A:92:ASP:OD1	1:A:96:LYS:NZ	2.50	0.45
1:C:60:LYS:N	1:C:61:PRO:HD3	2.31	0.45
1:D:60:LYS:N	1:D:61:PRO:HD3	2.31	0.45
1:B:80:ARG:HD2	1:B:135:ASN:HD21	1.82	0.45
1:D:50:GLU:O	1:D:54:LYS:HG3	2.16	0.45
1:C:92:ASP:OD1	1:C:96:LYS:NZ	2.49	0.45
1:B:109:THR:HG23	1:C:112:PHE:CZ	2.52	0.44
1:D:92:ASP:OD1	1:D:96:LYS:NZ	2.51	0.44
1:A:181:GLY:CA	1:B:89:ARG:NH1	2.80	0.43
1:D:160:LYS:HG3	2:D:312:HOH:O	2.17	0.43
1:A:130:PRO:HG2	1:A:187:MET:HE1	2.00	0.43
1:C:32:GLY:HA3	2:C:295:HOH:O	2.19	0.43
1:A:43:VAL:CG1	1:A:141:LEU:HD13	2.49	0.43
1:D:208:LEU:CB	2:D:209:HOH:O	2.54	0.43
1:B:112:PHE:CE1	1:C:109:THR:HG23	2.52	0.42
1:D:49:LYS:HG3	1:D:148:LEU:HD13	2.01	0.42
1:A:178:ILE:HD13	1:C:131:ALA:O	2.19	0.42
1:B:16:ILE:HG12	2:B:243:HOH:O	2.19	0.42
1:C:161:MET:HE2	2:C:342:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HB3	1:A:30:LYS:HZ2	1.84	0.42
1:A:80:ARG:HD2	1:A:135:ASN:HD21	1.83	0.42
1:B:43:VAL:CG1	1:B:141:LEU:HD13	2.49	0.42
1:B:130:PRO:HG2	1:B:187:MET:HE1	2.02	0.42
1:C:80:ARG:HD2	1:C:135:ASN:HD21	1.83	0.42
1:D:123:LYS:HE2	1:D:127:ARG:HH12	1.84	0.42
1:D:130:PRO:HG2	1:D:187:MET:HE1	2.02	0.42
1:B:115:LEU:CD1	1:B:163:GLY:HA3	2.49	0.42
1:C:43:VAL:CG1	1:C:141:LEU:HD13	2.49	0.42
1:A:123:LYS:HE2	1:A:127:ARG:HH12	1.84	0.42
1:B:47:LYS:HE3	1:B:47:LYS:HB2	1.90	0.42
1:A:115:LEU:CD1	1:A:163:GLY:HA3	2.50	0.41
1:B:178:ILE:HD13	1:D:131:ALA:O	2.20	0.41
1:B:182:GLN:CG	1:B:183:VAL:N	2.83	0.41
1:D:123:LYS:NZ	2:D:315:HOH:O	2.53	0.41
1:D:43:VAL:CG1	1:D:141:LEU:HD13	2.51	0.41
1:D:80:ARG:HD2	1:D:135:ASN:HD21	1.83	0.41
1:B:83:VAL:CG2	1:B:139:LEU:CD2	2.99	0.41
1:C:130:PRO:HG2	1:C:187:MET:HE1	2.03	0.41
1:A:83:VAL:CG2	1:A:139:LEU:CD2	2.99	0.41
1:B:123:LYS:HE2	1:B:127:ARG:HH12	1.85	0.41
1:D:83:VAL:CG2	1:D:139:LEU:CD2	2.99	0.41
1:D:115:LEU:CD1	1:D:163:GLY:HA3	2.51	0.40
1:C:122:LYS:HD2	1:C:122:LYS:O	2.21	0.40
1:A:182:GLN:CG	1:A:183:VAL:N	2.84	0.40
1:D:182:GLN:CG	1:D:183:VAL:N	2.84	0.40
1:B:81:ILE:HD11	1:B:110:ALA:HB1	2.03	0.40
1:B:183:VAL:HG11	1:D:75:ALA:HB2	2.03	0.40
1:C:101:GLU:HG2	2:C:332:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASP:OD2	1:D:206:GLU:O[4_555]	1.99	0.21

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	A	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
1	B	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
1	C	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
1	D	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
All	All	824/832 (99%)	792 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	173/173 (100%)	167 (96%)	6 (4%)	32	32
1	B	173/173 (100%)	167 (96%)	6 (4%)	32	32
1	C	173/173 (100%)	167 (96%)	6 (4%)	32	32
1	D	173/173 (100%)	167 (96%)	6 (4%)	32	32
All	All	692/692 (100%)	668 (96%)	24 (4%)	32	32

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

Mol	Chain	Res	Type
1	A	15	LYS
1	A	52	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	LEU
1	A	73	ARG
1	A	133	ILE
1	A	141	LEU
1	B	15	LYS
1	B	52	LEU
1	B	69	LEU
1	B	73	ARG
1	B	133	ILE
1	B	141	LEU
1	C	15	LYS
1	C	52	LEU
1	C	69	LEU
1	C	73	ARG
1	C	133	ILE
1	C	141	LEU
1	D	15	LYS
1	D	52	LEU
1	D	69	LEU
1	D	73	ARG
1	D	133	ILE
1	D	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	135	ASN
1	A	152	HIS
1	B	93	ASN
1	B	135	ASN
1	B	152	HIS
1	B	182	GLN
1	C	93	ASN
1	C	135	ASN
1	C	152	HIS
1	C	182	GLN
1	D	93	ASN
1	D	135	ASN
1	D	182	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.