Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 01:19 PM EST

PDB ID	:	1BAR
Title	:	THREE-DIMENSIONAL STRUCTURES OF ACIDIC AND BASIC FIBROBLAST GROWTH FACTORS
Authors	:	Zhu, X.; Komiya, H.; Chirino, A.; Faham, S.; Fox, G.M.; Arakawa, T.; Hsu, B.T.; Rees, D.C.
Deposited on	:	1992-09-29
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 (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:

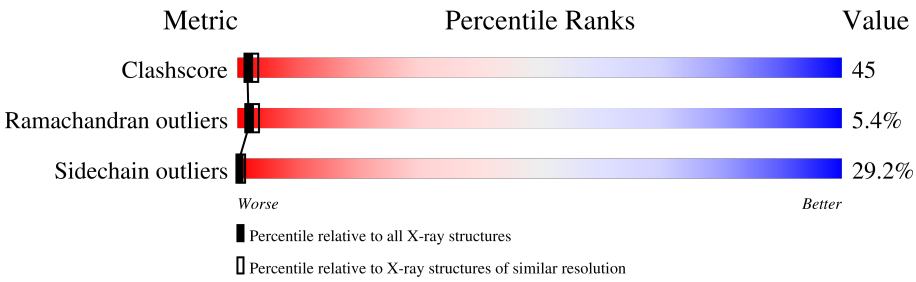
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	140	16% 34% 31% 11% 9%
1	B	140	20% 41% 25% 12% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2086 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 ACIDIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	994	638	171	182	3	0	0	0
			Total	C	N	O	S			
1	B	138	1056	680	179	194	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	conflict	UNP P03968
A	93	GLY	HIS	conflict	UNP P03968
B	47	ALA	CYS	conflict	UNP P03968
B	93	GLY	HIS	conflict	UNP P03968

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	23	23	23	0	0
			Total	O		
2	B	13	13	13	0	0

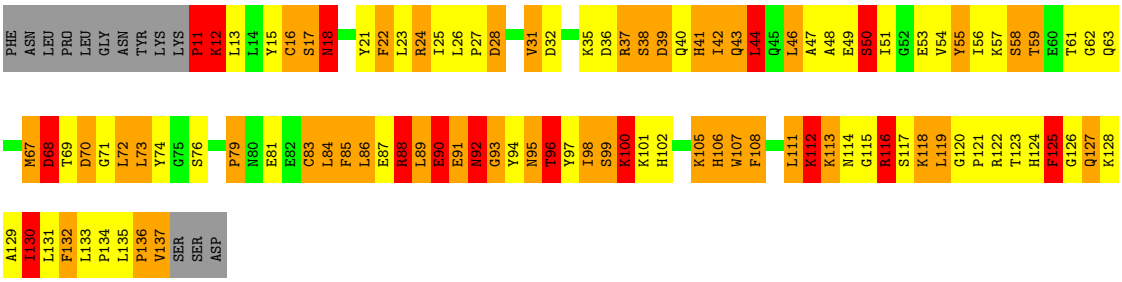
3 Residue-property plots (i)

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.

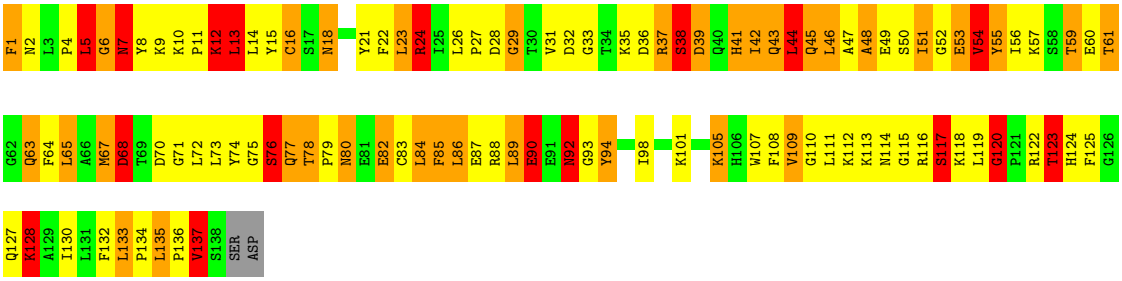
• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A: 16% 34% 31% 11% 9%



• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain B: 20% 41% 25% 12%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.60Å 78.60Å 115.90Å 90.00° 90.00° 120.00°	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}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2086	wwPDB-VP
Average B, all atoms ($Å^2$)	25.0	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	0.87	0/1017	1.40	6/1372 (0.4%)
1	B	0.80	1/1081 (0.1%)	1.35	3/1463 (0.2%)
All	All	0.83	1/2098 (0.0%)	1.38	9/2835 (0.3%)

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	72
1	B	0	76
All	All	0	148

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	TRP	CG-CD2	-5.22	1.34	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	B	107	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B	107	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	107	TRP	CE2-CD2-CG	-6.42	102.16	107.30
1	B	24	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	A	18	ASN	O-C-N	-6.10	112.83	123.20
1	A	68	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	18	ASN	C-N-CA	-5.82	110.07	122.30
1	A	11	PRO	N-CA-CB	5.17	109.50	103.30

There are no chirality outliers.

All (148) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LYS	Mainchain
1	A	105	LYS	Mainchain
1	A	106	HIS	Mainchain
1	A	107	TRP	Mainchain
1	A	108	PHE	Mainchain
1	A	11	PRO	Mainchain
1	A	111	LEU	Mainchain
1	A	112	LYS	Mainchain
1	A	115	GLY	Mainchain
1	A	116	ARG	Mainchain
1	A	117	SER	Mainchain
1	A	119	LEU	Mainchain
1	A	12	LYS	Mainchain
1	A	125	PHE	Mainchain
1	A	126	GLY	Mainchain
1	A	127	GLN	Mainchain
1	A	128	LYS	Mainchain
1	A	129	ALA	Mainchain
1	A	130	ILE	Mainchain
1	A	132	PHE	Mainchain
1	A	134	PRO	Mainchain
1	A	136	PRO	Mainchain
1	A	15	TYR	Mainchain
1	A	16	CYS	Mainchain
1	A	17	SER	Mainchain
1	A	18	ASN	Mainchain
1	A	21	TYR	Mainchain
1	A	22	PHE	Mainchain
1	A	23	LEU	Mainchain
1	A	24	ARG	Mainchain
1	A	28	ASP	Sidechain
1	A	32	ASP	Mainchain
1	A	35	LYS	Mainchain
1	A	36	ASP	Sidechain,Mainchain
1	A	37	ARG	Mainchain
1	A	38	SER	Mainchain
1	A	39	ASP	Mainchain
1	A	40	GLN	Mainchain
1	A	41	HIS	Mainchain
1	A	43	GLN	Mainchain
1	A	44	LEU	Mainchain
1	A	46	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	47	ALA	Mainchain
1	A	48	ALA	Mainchain
1	A	50	SER	Mainchain
1	A	53	GLU	Mainchain
1	A	54	VAL	Mainchain
1	A	55	TYR	Mainchain
1	A	58	SER	Mainchain
1	A	59	THR	Mainchain
1	A	62	GLY	Mainchain
1	A	63	GLN	Mainchain
1	A	67	MET	Mainchain
1	A	68	ASP	Mainchain
1	A	69	THR	Mainchain
1	A	70	ASP	Mainchain
1	A	72	LEU	Mainchain
1	A	74	TYR	Mainchain
1	A	79	PRO	Mainchain
1	A	81	GLU	Mainchain
1	A	83	CYS	Mainchain
1	A	84	LEU	Mainchain
1	A	85	PHE	Mainchain
1	A	88	ARG	Mainchain
1	A	89	LEU	Mainchain
1	A	91	GLU	Sidechain
1	A	92	ASN	Mainchain
1	A	93	GLY	Mainchain
1	A	95	ASN	Mainchain
1	A	96	THR	Mainchain
1	A	98	ILE	Mainchain
1	B	10	LYS	Mainchain
1	B	101	LYS	Mainchain
1	B	105	LYS	Mainchain
1	B	109	VAL	Mainchain
1	B	110	GLY	Mainchain
1	B	112	LYS	Mainchain
1	B	113	LYS	Mainchain
1	B	114	ASN	Mainchain
1	B	115	GLY	Mainchain
1	B	116	ARG	Mainchain
1	B	117	SER	Mainchain
1	B	118	LYS	Mainchain
1	B	12	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	B	120	GLY	Mainchain
1	B	122	ARG	Mainchain
1	B	123	THR	Mainchain
1	B	124	HIS	Mainchain
1	B	125	PHE	Mainchain
1	B	127	GLN	Mainchain
1	B	128	LYS	Mainchain
1	B	13	LEU	Mainchain
1	B	130	ILE	Mainchain
1	B	133	LEU	Mainchain
1	B	134	PRO	Mainchain
1	B	137	VAL	Mainchain
1	B	16	CYS	Mainchain
1	B	18	ASN	Mainchain
1	B	2	ASN	Mainchain
1	B	21	TYR	Mainchain
1	B	28	ASP	Mainchain
1	B	29	GLY	Mainchain
1	B	31	VAL	Mainchain
1	B	33	GLY	Mainchain
1	B	38	SER	Mainchain
1	B	39	ASP	Mainchain
1	B	41	HIS	Mainchain
1	B	43	GLN	Mainchain
1	B	44	LEU	Mainchain
1	B	45	GLN	Mainchain
1	B	46	LEU	Mainchain
1	B	48	ALA	Mainchain
1	B	5	LEU	Mainchain
1	B	50	SER	Mainchain
1	B	52	GLY	Mainchain
1	B	53	GLU	Sidechain,Mainchain
1	B	54	VAL	Mainchain
1	B	55	TYR	Mainchain
1	B	56	ILE	Mainchain
1	B	57	LYS	Mainchain
1	B	59	THR	Mainchain
1	B	60	GLU	Mainchain
1	B	63	GLN	Mainchain
1	B	64	PHE	Mainchain
1	B	65	LEU	Mainchain
1	B	67	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	B	68	ASP	Mainchain
1	B	7	ASN	Mainchain
1	B	71	GLY	Mainchain
1	B	75	GLY	Mainchain
1	B	76	SER	Mainchain
1	B	77	GLN	Mainchain
1	B	78	THR	Mainchain
1	B	79	PRO	Mainchain
1	B	80	ASN	Mainchain
1	B	82	GLU	Mainchain
1	B	84	LEU	Mainchain
1	B	85	PHE	Mainchain
1	B	86	LEU	Mainchain
1	B	87	GLU	Mainchain
1	B	89	LEU	Mainchain
1	B	90	GLU	Sidechain
1	B	92	ASN	Mainchain
1	B	93	GLY	Mainchain
1	B	94	TYR	Sidechain,Mainchain

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	994	0	980	95	0
1	B	1056	0	1006	93	0
2	A	23	0	0	0	0
2	B	13	0	0	1	0
All	All	2086	0	1986	180	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 45.

All (180) 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:37:ARG:HH11	1:B:37:ARG:HG3	1.19	1.06
1:A:123:THR:HB	1:A:130:ILE:HD11	1.40	1.03
1:A:68:ASP:HB2	1:A:72:LEU:H	1.30	0.97
1:B:39:ASP:HB3	1:B:42:ILE:HG23	1.48	0.95
1:A:93:GLY:HA3	1:B:7:ASN:HB3	1.61	0.83
1:B:68:ASP:HB2	1:B:72:LEU:H	1.44	0.83
1:B:108:PHE:HD2	1:B:123:THR:HG23	1.43	0.83
1:A:46:LEU:HD23	1:A:56:ILE:HG12	1.60	0.83
1:A:118:LYS:HD3	1:A:123:THR:HG22	1.62	0.81
1:A:46:LEU:CD2	1:A:56:ILE:HG12	2.11	0.80
1:A:123:THR:CB	1:A:130:ILE:HD11	2.11	0.80
1:A:87:GLU:HG3	1:A:97:TYR:CE1	2.15	0.80
1:B:39:ASP:HB3	1:B:42:ILE:CG2	2.12	0.80
1:A:123:THR:HB	1:A:130:ILE:CD1	2.10	0.80
1:B:47:ALA:O	1:B:54:VAL:HG22	1.83	0.77
1:B:24:ARG:NH1	1:B:26:LEU:HD21	2.00	0.77
1:B:37:ARG:HG3	1:B:37:ARG:NH1	1.95	0.76
1:B:61:THR:OG1	1:B:63:GLN:HG3	1.85	0.76
1:A:68:ASP:HB3	1:A:70:ASP:H	1.50	0.76
1:A:106:HIS:CD2	1:B:89:LEU:HD21	2.21	0.75
1:B:4:PRO:O	1:B:6:GLY:N	2.19	0.75
1:B:24:ARG:HG2	1:B:32:ASP:OD1	1.87	0.74
1:B:120:GLY:O	1:B:123:THR:HB	1.87	0.74
1:A:11:PRO:HB2	1:A:137:VAL:HG21	1.71	0.73
1:A:16:CYS:HB2	1:A:132:PHE:CE2	2.24	0.72
1:B:68:ASP:HB3	1:B:70:ASP:H	1.53	0.72
1:A:13:LEU:HD22	1:A:42:ILE:HG13	1.72	0.72
1:A:108:PHE:CB	1:A:130:ILE:HG12	2.19	0.72
1:A:55:TYR:CZ	1:A:84:LEU:CD1	2.72	0.72
1:B:108:PHE:H	1:B:123:THR:HG21	1.55	0.70
1:B:108:PHE:HD2	1:B:123:THR:CG2	2.04	0.70
1:A:123:THR:CG2	1:A:130:ILE:HD11	2.23	0.69
1:B:24:ARG:NH1	1:B:26:LEU:HD11	2.08	0.69
1:A:11:PRO:HB2	1:A:137:VAL:CG2	2.23	0.68
1:A:24:ARG:HD3	1:A:26:LEU:HG	1.75	0.68
1:B:94:TYR:CE2	1:B:133:LEU:HB2	2.30	0.66
1:A:37:ARG:CZ	1:B:1:PHE:HB3	2.27	0.65
1:B:48:ALA:HA	1:B:54:VAL:HG23	1.77	0.65
1:A:49:GLU:O	1:A:50:SER:CB	2.45	0.64
1:B:92:ASN:ND2	1:B:92:ASN:H	1.94	0.64
1:A:114:ASN:OD1	1:A:114:ASN:C	2.34	0.63
1:A:133:LEU:HD21	1:B:4:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASN:HB2	1:B:128:LYS:HB3	1.81	0.62
1:A:88:ARG:HD3	1:A:96:THR:HG21	1.82	0.62
1:B:24:ARG:HD2	1:B:26:LEU:HD21	1.82	0.62
1:A:55:TYR:CZ	1:A:84:LEU:HD12	2.35	0.62
1:A:108:PHE:HB2	1:A:130:ILE:HG12	1.81	0.61
1:B:51:ILE:N	1:B:51:ILE:HD13	2.15	0.61
1:A:85:PHE:CD1	1:A:99:SER:HA	2.34	0.61
1:A:119:LEU:C	1:A:121:PRO:HD2	2.20	0.61
1:A:119:LEU:HB3	1:A:121:PRO:HD2	1.83	0.61
1:A:124:HIS:HD2	1:A:125:PHE:O	1.84	0.60
1:A:120:GLY:N	1:A:121:PRO:CD	2.63	0.59
1:A:27:PRO:HG3	1:A:41:HIS:CE1	2.38	0.59
1:A:25:ILE:HG13	1:A:44:LEU:HD21	1.82	0.59
1:B:14:LEU:HD12	1:B:23:LEU:HD23	1.85	0.59
1:A:12:LYS:HG3	1:A:135:LEU:O	2.03	0.59
1:A:88:ARG:CD	1:A:96:THR:CG2	2.81	0.58
1:B:68:ASP:CG	1:B:72:LEU:HB3	2.23	0.58
1:A:49:GLU:HB2	1:A:55:TYR:CE2	2.38	0.58
1:A:92:ASN:O	1:B:7:ASN:HB2	2.03	0.58
1:B:4:PRO:HB2	1:B:7:ASN:OD1	2.02	0.58
1:B:92:ASN:OD1	1:B:94:TYR:HB2	2.03	0.58
1:B:36:ASP:O	1:B:38:SER:N	2.37	0.57
1:B:68:ASP:OD2	1:B:72:LEU:HB3	2.04	0.56
1:A:46:LEU:HD23	1:A:56:ILE:CG1	2.33	0.56
1:B:36:ASP:C	1:B:38:SER:H	2.09	0.56
1:B:92:ASN:ND2	1:B:92:ASN:N	2.52	0.56
1:A:55:TYR:CE1	1:A:84:LEU:HD12	2.40	0.56
1:A:119:LEU:O	1:A:120:GLY:C	2.42	0.56
1:B:16:CYS:HB2	1:B:132:PHE:CE2	2.42	0.55
1:A:137:VAL:HG13	1:A:137:VAL:O	2.06	0.55
1:A:17:SER:HB2	1:A:94:TYR:CE2	2.43	0.54
1:B:43:GLN:HE21	1:B:137:VAL:HG11	1.72	0.54
1:B:80:ASN:OD1	1:B:82:GLU:HG3	2.07	0.54
1:A:26:LEU:HB3	1:A:27:PRO:CD	2.37	0.54
1:B:24:ARG:HH11	1:B:26:LEU:HD21	1.73	0.54
1:B:24:ARG:HD2	1:B:26:LEU:CD2	2.37	0.54
1:A:90:GLU:HA	1:A:90:GLU:OE1	2.07	0.53
1:B:11:PRO:O	1:B:12:LYS:HG3	2.08	0.53
1:A:92:ASN:O	1:B:7:ASN:CB	2.56	0.53
1:A:91:GLU:C	1:A:93:GLY:H	2.12	0.53
1:A:91:GLU:C	1:A:93:GLY:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HG2	1:A:55:TYR:HE2	1.73	0.52
1:A:49:GLU:CG	1:A:55:TYR:HE2	2.22	0.52
1:A:124:HIS:O	1:A:125:PHE:C	2.47	0.52
1:A:88:ARG:CD	1:A:96:THR:HG21	2.39	0.51
1:B:18:ASN:HB2	1:B:128:LYS:C	2.30	0.51
1:A:119:LEU:O	1:A:121:PRO:HD2	2.10	0.51
1:A:46:LEU:HD21	1:A:56:ILE:HG12	1.90	0.51
1:B:24:ARG:HH12	1:B:26:LEU:HD11	1.74	0.51
1:A:39:ASP:OD1	1:A:41:HIS:HB2	2.10	0.51
1:A:108:PHE:HB2	1:A:130:ILE:CG1	2.40	0.51
1:B:94:TYR:CD2	1:B:133:LEU:HB2	2.47	0.50
1:A:67:MET:HG2	1:A:71:GLY:HA2	1.93	0.50
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.02	0.50
1:B:13:LEU:CD1	1:B:137:VAL:HG13	2.41	0.50
1:B:44:LEU:HA	1:B:59:THR:HG23	1.92	0.50
1:A:90:GLU:HB2	1:A:94:TYR:O	2.12	0.50
1:B:13:LEU:HD13	1:B:137:VAL:HA	1.94	0.49
1:A:118:LYS:HD3	1:A:123:THR:CG2	2.39	0.49
1:B:38:SER:O	1:B:39:ASP:C	2.50	0.49
1:B:90:GLU:HB2	1:B:94:TYR:O	2.11	0.49
1:B:26:LEU:HB3	1:B:27:PRO:HD2	1.94	0.49
1:A:88:ARG:CD	1:A:96:THR:HG22	2.42	0.49
1:B:119:LEU:O	1:B:120:GLY:C	2.51	0.49
1:A:12:LYS:HG3	1:A:136:PRO:HA	1.95	0.49
1:A:13:LEU:HB3	1:A:22:PHE:CD1	2.47	0.48
1:A:67:MET:CG	1:A:71:GLY:HA2	2.42	0.48
1:A:18:ASN:HD21	1:A:113:LYS:NZ	2.11	0.48
1:A:88:ARG:HD3	1:A:96:THR:CG2	2.42	0.48
1:B:108:PHE:CD2	1:B:123:THR:HG23	2.35	0.48
1:B:26:LEU:HB3	1:B:27:PRO:CD	2.43	0.48
1:A:24:ARG:HD3	1:A:26:LEU:CG	2.43	0.48
1:B:5:LEU:O	1:B:6:GLY:C	2.50	0.48
1:B:51:ILE:N	1:B:51:ILE:CD1	2.77	0.48
1:A:108:PHE:CB	1:A:130:ILE:CG1	2.90	0.48
1:B:36:ASP:C	1:B:38:SER:N	2.67	0.48
1:B:68:ASP:OD2	1:B:72:LEU:HD23	2.14	0.48
1:B:111:LEU:HD23	1:B:117:SER:HA	1.95	0.47
1:A:112:LYS:HG3	1:A:116:ARG:O	2.14	0.47
1:B:13:LEU:HD23	1:B:22:PHE:CE1	2.50	0.47
1:B:73:LEU:HD13	2:B:512:HOH:O	2.13	0.47
1:B:37:ARG:NH1	1:B:37:ARG:CG	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:PRO:C	1:B:12:LYS:HG3	2.35	0.46
1:B:61:THR:HG1	1:B:63:GLN:CG	2.29	0.46
1:A:86:LEU:O	1:A:97:TYR:HA	2.16	0.46
1:B:73:LEU:HD11	1:B:109:VAL:HA	1.97	0.46
1:B:61:THR:OG1	1:B:63:GLN:CG	2.60	0.46
1:A:79:PRO:HA	1:A:83:CYS:SG	2.56	0.45
1:A:124:HIS:O	1:A:127:GLN:HB2	2.17	0.45
1:B:4:PRO:O	1:B:5:LEU:C	2.52	0.45
1:B:22:PHE:CG	1:B:42:ILE:HD12	2.51	0.45
1:A:95:ASN:ND2	1:A:95:ASN:N	2.64	0.45
1:A:55:TYR:OH	1:A:84:LEU:CD1	2.65	0.45
1:A:106:HIS:CD2	1:B:89:LEU:CD2	2.94	0.45
1:A:37:ARG:NH1	1:B:1:PHE:HB3	2.31	0.45
1:B:74:TYR:CE2	1:B:76:SER:HB2	2.50	0.45
1:A:24:ARG:HD3	1:A:26:LEU:CD2	2.46	0.45
1:A:31:VAL:HG11	1:A:73:LEU:HB3	1.97	0.45
1:A:112:LYS:HE3	1:A:116:ARG:HB2	1.99	0.45
1:A:95:ASN:N	1:A:95:ASN:HD22	2.15	0.45
1:A:12:LYS:CG	1:A:135:LEU:O	2.65	0.44
1:B:53:GLU:HA	1:B:85:PHE:O	2.18	0.44
1:A:31:VAL:HG13	1:A:73:LEU:O	2.18	0.44
1:A:92:ASN:OD1	1:A:92:ASN:N	2.51	0.44
1:B:29:GLY:HA2	1:B:63:GLN:HE22	1.83	0.44
1:B:98:ILE:HG13	1:B:108:PHE:CD1	2.53	0.43
1:A:18:ASN:HD22	1:A:18:ASN:HA	1.61	0.43
1:B:15:TYR:O	1:B:132:PHE:HA	2.18	0.43
1:B:76:SER:OG	1:B:78:THR:O	2.35	0.43
1:A:11:PRO:O	1:A:137:VAL:HB	2.18	0.43
1:A:13:LEU:CD2	1:A:42:ILE:HG13	2.46	0.43
1:A:88:ARG:HD2	1:A:96:THR:CG2	2.49	0.43
1:B:7:ASN:C	1:B:9:LYS:N	2.71	0.43
1:B:55:TYR:C	1:B:55:TYR:CD1	2.92	0.42
1:B:98:ILE:HG13	1:B:108:PHE:CE1	2.54	0.42
1:A:88:ARG:HD2	1:A:98:ILE:CD1	2.49	0.42
1:A:17:SER:HB2	1:A:94:TYR:HE2	1.85	0.42
1:A:100:LYS:C	1:A:102:HIS:N	2.72	0.42
1:B:108:PHE:N	1:B:123:THR:HG21	2.28	0.42
1:B:18:ASN:CB	1:B:128:LYS:HB3	2.48	0.42
1:B:39:ASP:OD1	1:B:41:HIS:N	2.51	0.42
1:A:86:LEU:HD22	1:A:86:LEU:HA	1.85	0.41
1:B:53:GLU:OE2	1:B:84:LEU:HD13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HD21	1:A:113:LYS:HZ2	1.68	0.41
1:B:13:LEU:O	1:B:135:LEU:N	2.48	0.41
1:A:135:LEU:HB3	1:A:136:PRO:CD	2.51	0.41
1:B:68:ASP:HB2	1:B:72:LEU:N	2.24	0.41
1:B:92:ASN:N	1:B:92:ASN:HD22	2.18	0.41
1:A:67:MET:HA	1:A:72:LEU:O	2.21	0.41
1:B:80:ASN:O	1:B:83:CYS:HB2	2.21	0.41
1:B:23:LEU:HA	1:B:111:LEU:HD11	2.03	0.40
1:A:116:ARG:H	1:A:116:ARG:HG2	1.74	0.40
1:B:135:LEU:HA	1:B:136:PRO:HD3	1.91	0.40
1:B:68:ASP:HB2	1:B:72:LEU:HB3	2.02	0.40
1:A:89:LEU:C	1:A:89:LEU:HD12	2.41	0.40
1:A:135:LEU:HB3	1:A:136:PRO:HD2	2.02	0.40
1:B:38:SER:C	1:B:39:ASP:O	2.57	0.40
1:B:61:THR:HG1	1:B:63:GLN:CD	2.23	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	125/140 (89%)	109 (87%)	9 (7%)	7 (6%)	2 3
1	B	136/140 (97%)	119 (88%)	10 (7%)	7 (5%)	2 3
All	All	261/280 (93%)	228 (87%)	19 (7%)	14 (5%)	2 3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	50	SER
1	A	68	ASP

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Mol	Chain	Res	Type
1	A	90	GLU
1	B	5	LEU
1	A	101	LYS
1	A	125	PHE
1	B	6	GLY
1	B	120	GLY
1	B	7	ASN
1	B	8	TYR
1	B	117	SER
1	A	116	ARG
1	B	68	ASP

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	104/121 (86%)	73 (70%)	31 (30%)	0 1
1	B	105/121 (87%)	75 (71%)	30 (29%)	0 1
All	All	209/242 (86%)	148 (71%)	61 (29%)	0 1

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	18	ASN
1	A	28	ASP
1	A	31	VAL
1	A	38	SER
1	A	42	ILE
1	A	43	GLN
1	A	44	LEU
1	A	51	ILE
1	A	57	LYS
1	A	58	SER
1	A	59	THR

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Mol	Chain	Res	Type
1	A	61	THR
1	A	73	LEU
1	A	76	SER
1	A	86	LEU
1	A	88	ARG
1	A	90	GLU
1	A	92	ASN
1	A	96	THR
1	A	99	SER
1	A	100	LYS
1	A	105	LYS
1	A	111	LEU
1	A	112	LYS
1	A	113	LYS
1	A	118	LYS
1	A	122	ARG
1	A	130	ILE
1	A	131	LEU
1	A	137	VAL
1	B	1	PHE
1	B	5	LEU
1	B	12	LYS
1	B	13	LEU
1	B	23	LEU
1	B	24	ARG
1	B	35	LYS
1	B	37	ARG
1	B	38	SER
1	B	42	ILE
1	B	44	LEU
1	B	45	GLN
1	B	46	LEU
1	B	49	GLU
1	B	51	ILE
1	B	54	VAL
1	B	61	THR
1	B	65	LEU
1	B	67	MET
1	B	76	SER
1	B	77	GLN
1	B	86	LEU
1	B	88	ARG

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Mol	Chain	Res	Type
1	B	90	GLU
1	B	92	ASN
1	B	105	LYS
1	B	123	THR
1	B	128	LYS
1	B	135	LEU
1	B	137	VAL

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	18	ASN
1	A	41	HIS
1	A	95	ASN
1	A	124	HIS
1	B	43	GLN
1	B	63	GLN
1	B	92	ASN
1	B	124	HIS

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.