



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:00 AM UTC

PDB ID : 1C4R / pdb_00001c4r
Title : THE STRUCTURE OF THE LIGAND-BINDING DOMAIN OF NEUREXIN 1BETA: REGULATION OF LNS DOMAIN FUNCTION BY ALTERNATIVE SPLICING
Authors : Rudenko, G.; Nguyen, T.; Chelliah, Y.; Sudhof, T.C.; Deisenhofer, J.
Deposited on : 1999-09-28
Resolution : 2.60 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

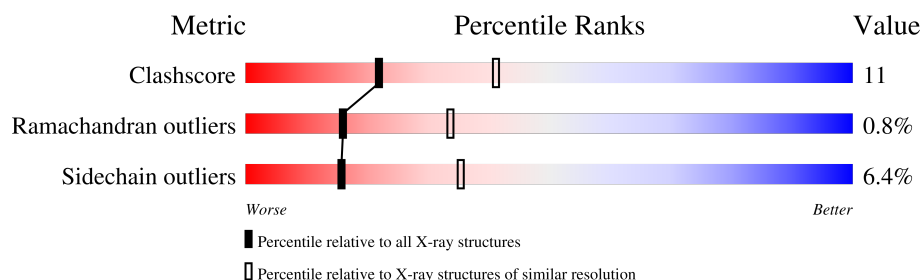
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	182	
1	B	182	
1	C	182	
1	D	182	
1	E	182	
1	F	182	
1	G	182	
1	H	182	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11086 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 NEUREXIN-I BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	14	0	0
			1379	869	246	263	1			
1	B	178	Total	C	N	O	S	15	0	0
			1363	859	244	259	1			
1	C	180	Total	C	N	O	S	19	0	0
			1379	869	246	263	1			
1	D	178	Total	C	N	O	S	15	0	0
			1363	859	244	259	1			
1	E	181	Total	C	N	O	S	21	0	0
			1386	874	247	264	1			
1	F	177	Total	C	N	O	S	20	0	0
			1359	857	243	258	1			
1	G	182	Total	C	N	O	S	10	0	0
			1390	876	248	265	1			
1	H	177	Total	C	N	O	S	14	0	0
			1359	857	243	258	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	19	Total	O	0	0
			19	19		
2	C	11	Total	O	0	0
			11	11		
2	D	21	Total	O	0	0
			21	21		
2	E	8	Total	O	0	0
			8	8		
2	F	14	Total	O	0	0
			14	14		

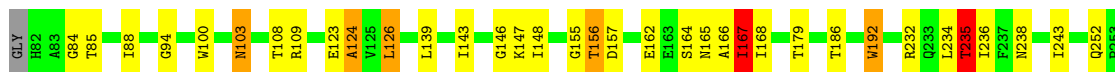
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	13	Total	O	0	0
			13	13		
2	H	14	Total	O	0	0
			14	14		

Note EDS was not executed.

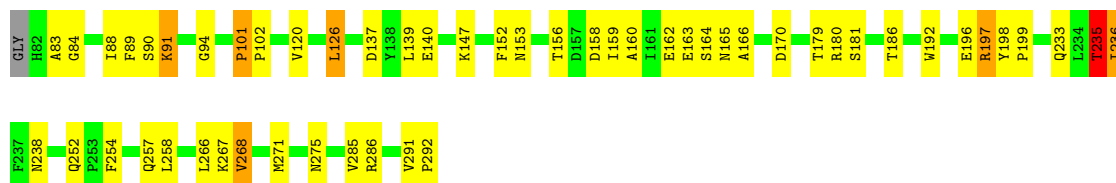
Chain A: 69% 27% ...





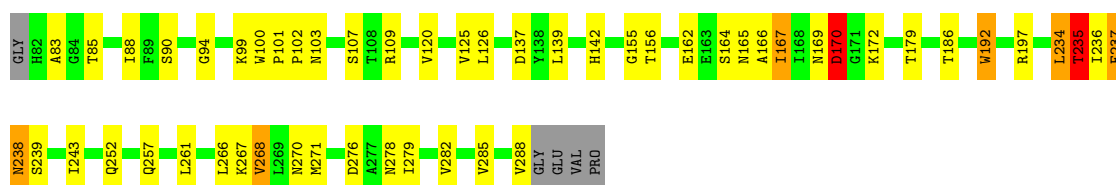
• Molecule 1: NEUREXIN-I BETA

Chain E: 70% 25% . .



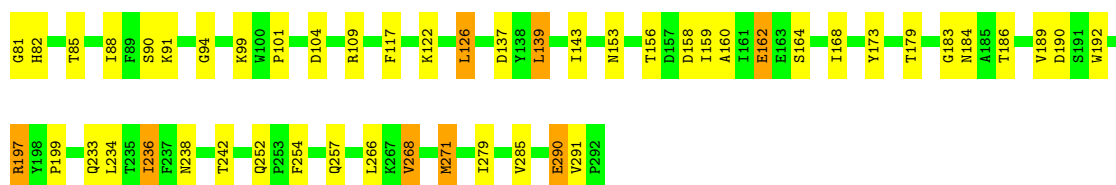
• Molecule 1: NEUREXIN-I BETA

Chain F: 68% 25% . . .



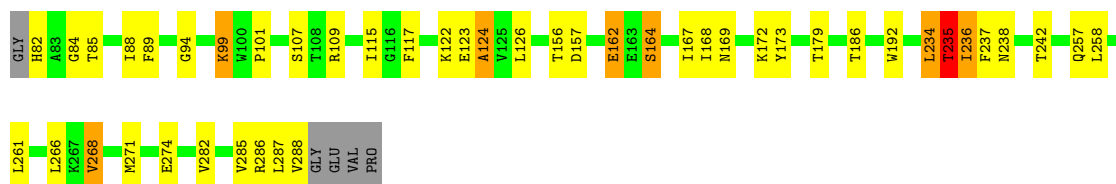
• Molecule 1: NEUREXIN-I BETA

Chain G: 73% 23% .



• Molecule 1: NEUREXIN-I BETA

Chain H: 72% 21% . . .



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 2	Depositor
Cell constants a, b, c, α , β , γ	116.60 Å 195.90 Å 103.61 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.9 (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11086	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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	0.74	0/1405	1.17	12/1904 (0.6%)
1	B	0.91	1/1389 (0.1%)	1.27	16/1882 (0.9%)
1	C	0.78	1/1405 (0.1%)	1.17	13/1904 (0.7%)
1	D	0.91	2/1389 (0.1%)	1.29	15/1882 (0.8%)
1	E	0.84	2/1413 (0.1%)	1.16	11/1916 (0.6%)
1	F	0.82	0/1385	1.30	21/1877 (1.1%)
1	G	0.94	1/1417 (0.1%)	1.19	7/1921 (0.4%)
1	H	0.83	0/1385	1.22	13/1877 (0.7%)
All	All	0.85	7/11188 (0.1%)	1.22	108/15163 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	271	MET	SD-CE	-7.55	1.60	1.79
1	D	271	MET	SD-CE	-7.28	1.61	1.79
1	E	120	VAL	CA-CB	6.75	1.61	1.54
1	D	268	VAL	CA-CB	6.62	1.61	1.54
1	C	271	MET	SD-CE	-5.33	1.66	1.79
1	B	165	ASN	CA-C	-5.29	1.47	1.53
1	E	180	ARG	CA-C	-5.25	1.46	1.52

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	ARG	N-CA-C	-12.44	92.06	110.48
1	H	238	ASN	N-CA-C	10.80	126.94	109.76
1	A	290	GLU	N-CA-C	10.47	125.83	107.61
1	B	100	TRP	CA-C-N	-9.86	110.23	120.38
1	B	100	TRP	C-N-CA	-9.86	110.23	120.38
1	F	192	TRP	CA-C-N	-9.66	110.10	119.76
1	F	192	TRP	C-N-CA	-9.66	110.10	119.76
1	D	268	VAL	N-CA-C	9.06	119.87	110.36
1	F	268	VAL	N-CA-C	8.32	119.10	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	THR	N-CA-C	8.18	124.35	113.72
1	H	236	ILE	N-CA-C	8.14	119.56	108.17
1	F	238	ASN	N-CA-C	8.10	122.27	110.28
1	B	268	VAL	N-CA-C	8.02	118.78	110.36
1	C	170	ASP	N-CA-C	7.91	121.74	112.72
1	G	238	ASN	N-CA-C	7.89	122.66	110.20
1	E	236	ILE	N-CA-C	7.64	119.48	108.48
1	H	235	THR	N-CA-CB	-7.62	100.92	110.98
1	F	234	LEU	N-CA-C	-7.52	100.39	110.55
1	C	234	LEU	N-CA-C	-7.49	100.44	110.55
1	H	234	LEU	N-CA-C	-7.43	99.48	110.48
1	C	101	PRO	CA-C-N	7.41	129.11	119.84
1	C	101	PRO	C-N-CA	7.41	129.11	119.84
1	D	100	TRP	CA-C-N	-7.27	112.89	120.38
1	D	100	TRP	C-N-CA	-7.27	112.89	120.38
1	H	268	VAL	N-CA-C	7.25	117.97	110.36
1	D	192	TRP	CA-C-N	-7.23	112.55	119.85
1	D	192	TRP	C-N-CA	-7.23	112.55	119.85
1	B	164	SER	N-CA-C	7.21	121.31	112.23
1	F	107	SER	N-CA-C	-7.19	97.68	109.40
1	F	235	THR	N-CA-CB	-7.15	101.49	111.00
1	A	268	VAL	N-CA-C	7.06	117.19	110.42
1	G	236	ILE	N-CA-C	6.88	117.81	108.17
1	A	236	ILE	N-CA-C	6.87	118.37	108.48
1	C	238	ASN	N-CA-C	6.85	121.21	110.32
1	F	236	ILE	N-CA-C	6.81	118.09	108.36
1	H	164	SER	N-CA-C	6.72	121.33	113.20
1	B	236	ILE	N-CA-C	6.70	117.55	108.17
1	E	268	VAL	N-CA-C	6.70	118.26	110.62
1	H	101	PRO	N-CA-C	-6.70	102.52	110.70
1	D	252	GLN	CA-C-N	6.70	127.10	119.93
1	D	252	GLN	C-N-CA	6.70	127.10	119.93
1	C	252	GLN	CA-C-N	6.67	127.07	119.93
1	C	252	GLN	C-N-CA	6.67	127.07	119.93
1	A	101	PRO	CA-C-N	6.64	128.14	119.84
1	A	101	PRO	C-N-CA	6.64	128.14	119.84
1	B	98	TYR	N-CA-C	-6.58	99.00	109.59
1	C	268	VAL	N-CA-C	6.58	118.12	110.62
1	H	274	GLU	N-CA-C	-6.57	104.85	112.92
1	D	236	ILE	N-CA-C	6.54	117.33	108.17
1	E	252	GLN	CA-C-N	6.31	126.68	119.93
1	E	252	GLN	C-N-CA	6.31	126.68	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	100	TRP	CA-C-N	-6.29	113.90	120.38
1	F	100	TRP	C-N-CA	-6.29	113.90	120.38
1	F	170	ASP	N-CA-C	6.24	124.09	110.80
1	E	140	GLU	N-CA-C	6.24	118.62	108.26
1	F	164	SER	N-CA-C	6.22	118.99	111.40
1	E	238	ASN	N-CA-C	6.19	119.98	110.20
1	D	164	SER	N-CA-C	6.17	120.97	113.38
1	B	169	ASN	N-CA-CB	-6.16	101.19	110.91
1	A	237	PHE	N-CA-C	-6.10	97.26	107.99
1	C	236	ILE	N-CA-C	6.01	116.52	108.11
1	E	84	GLY	N-CA-C	-6.01	104.64	111.85
1	G	268	VAL	N-CA-C	5.97	116.63	110.36
1	B	122	LYS	N-CA-C	-5.94	105.12	112.90
1	F	252	GLN	CA-C-N	5.85	125.87	119.90
1	F	252	GLN	C-N-CA	5.85	125.87	119.90
1	E	235	THR	N-CA-CB	-5.83	102.84	110.88
1	G	158	ASP	N-CA-C	-5.77	100.59	109.76
1	H	286	ARG	N-CA-C	5.75	117.80	108.26
1	B	158	ASP	N-CA-C	-5.71	100.68	109.76
1	F	267	LYS	N-CA-C	-5.68	101.70	109.71
1	F	243	ILE	N-CA-C	-5.64	98.32	107.28
1	G	252	GLN	CA-C-N	5.62	125.64	119.90
1	G	252	GLN	C-N-CA	5.62	125.64	119.90
1	D	238	ASN	N-CA-C	5.62	119.08	110.20
1	F	101	PRO	CA-C-N	5.62	126.86	119.84
1	F	101	PRO	C-N-CA	5.62	126.86	119.84
1	D	243	ILE	N-CA-C	-5.60	99.57	107.75
1	B	238	ASN	N-CA-C	5.59	119.04	110.20
1	B	101	PRO	CA-C-N	5.54	126.76	119.84
1	B	101	PRO	C-N-CA	5.54	126.76	119.84
1	E	267	LYS	N-CA-C	-5.54	101.90	109.71
1	C	185	ALA	N-CA-C	5.51	117.56	109.24
1	F	237	PHE	N-CA-C	-5.46	98.38	107.99
1	D	167	ILE	N-CA-C	-5.40	101.24	109.78
1	H	115	ILE	N-CA-C	5.39	114.96	108.06
1	B	243	ILE	N-CA-C	-5.38	98.72	107.28
1	C	100	TRP	CA-C-N	-5.34	114.88	120.38
1	C	100	TRP	C-N-CA	-5.34	114.88	120.38
1	G	234	LEU	N-CA-C	-5.34	103.48	110.53
1	A	235	THR	N-CA-CB	-5.31	102.85	110.65
1	E	286	ARG	N-CA-C	5.29	118.07	109.24
1	D	108	THR	N-CA-C	5.24	117.35	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	276	ASP	N-CA-C	-5.21	103.47	110.24
1	C	131	SER	N-CA-C	-5.19	103.83	110.53
1	H	107	SER	N-CA-C	-5.19	100.57	109.24
1	A	274	GLU	N-CA-C	-5.16	107.15	112.93
1	E	158	ASP	N-CA-C	-5.15	101.57	109.76
1	F	83	ALA	N-CA-C	5.13	116.99	109.24
1	H	237	PHE	N-CA-C	-5.09	100.21	108.41
1	A	252	GLN	CA-C-N	5.08	125.08	119.90
1	A	252	GLN	C-N-CA	5.08	125.08	119.90
1	B	101	PRO	N-CA-C	-5.08	104.51	110.70
1	B	237	PHE	N-CA-C	-5.03	99.14	107.99
1	A	167	ILE	N-CA-C	-5.02	100.67	108.95
1	H	122	LYS	N-CA-C	-5.02	107.33	113.50
1	B	107	SER	N-CA-C	-5.01	100.87	109.24
1	D	235	THR	N-CA-C	5.01	121.09	114.12

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	1379	0	1365	32	0
1	B	1363	0	1350	29	0
1	C	1379	0	1365	26	0
1	D	1363	0	1350	30	0
1	E	1386	0	1372	33	0
1	F	1359	0	1347	31	0
1	G	1390	0	1375	30	0
1	H	1359	0	1347	26	0
2	A	8	0	0	0	0
2	B	19	0	0	0	0
2	C	11	0	0	1	0
2	D	21	0	0	1	0
2	E	8	0	0	0	0
2	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	13	0	0	0	0
2	H	14	0	0	0	0
All	All	11086	0	10871	231	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 11.

All (231) 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:C:156:THR:HB	1:C:233:GLN:HG3	1.38	1.04
1:H:109:ARG:HG2	1:H:235:THR:HG23	1.49	0.94
1:C:266:LEU:HB3	1:C:271:MET:HE1	1.49	0.94
1:A:192:TRP:HB3	1:A:193:PRO:HD2	1.49	0.92
1:D:266:LEU:HB3	1:D:271:MET:HE1	1.47	0.92
1:E:266:LEU:HB3	1:E:271:MET:HE1	1.51	0.92
1:G:266:LEU:HB3	1:G:271:MET:HE1	1.53	0.91
1:B:120:VAL:C	1:B:169:ASN:HD21	1.79	0.90
1:D:166:ALA:HB3	1:D:192:TRP:CZ3	2.06	0.90
1:B:266:LEU:HB3	1:B:271:MET:HE1	1.54	0.89
1:A:266:LEU:HB3	1:A:271:MET:HE1	1.57	0.87
1:G:290:GLU:H	1:G:290:GLU:CD	1.82	0.87
1:B:268:VAL:HA	1:B:271:MET:HE3	1.61	0.83
1:F:266:LEU:HB3	1:F:271:MET:HE1	1.58	0.83
1:D:268:VAL:HA	1:D:271:MET:HE3	1.59	0.83
1:D:94:GLY:HA3	1:D:285:VAL:HG23	1.62	0.82
1:E:235:THR:HG22	1:E:236:ILE:HG13	1.62	0.81
1:H:266:LEU:HB3	1:H:271:MET:HE1	1.60	0.81
1:B:166:ALA:CB	1:B:192:TRP:CZ3	2.65	0.79
1:H:268:VAL:HA	1:H:271:MET:HE3	1.63	0.79
1:F:94:GLY:HA3	1:F:285:VAL:HG23	1.64	0.79
1:E:291:VAL:HG13	1:E:292:PRO:HD2	1.65	0.79
1:C:268:VAL:HA	1:C:271:MET:HE3	1.64	0.78
1:G:268:VAL:HA	1:G:271:MET:HE3	1.66	0.77
1:D:94:GLY:HA3	1:D:285:VAL:CG2	2.14	0.77
1:H:94:GLY:HA3	1:H:285:VAL:HG23	1.66	0.77
1:B:120:VAL:C	1:B:169:ASN:ND2	2.43	0.77
1:D:103:ASN:N	1:D:103:ASN:HD22	1.80	0.77
1:A:94:GLY:HA3	1:A:285:VAL:HG23	1.67	0.76
1:A:268:VAL:HA	1:A:271:MET:HE3	1.67	0.75
1:E:268:VAL:HA	1:E:271:MET:HE3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ALA:HB3	1:A:192:TRP:CZ3	2.21	0.74
1:G:94:GLY:HA3	1:G:285:VAL:HG23	1.70	0.74
1:G:88:ILE:HG12	1:G:257:GLN:HG2	1.71	0.73
1:D:109:ARG:HD3	1:D:235:THR:HG21	1.69	0.73
1:F:268:VAL:HA	1:F:271:MET:HE3	1.69	0.72
1:E:166:ALA:HB3	1:E:192:TRP:CZ3	2.24	0.72
1:E:291:VAL:CG1	1:E:292:PRO:HD2	2.20	0.72
1:B:166:ALA:HB1	1:B:192:TRP:CZ3	2.25	0.71
1:H:117:PHE:CE1	1:H:168:ILE:HD13	2.25	0.71
1:D:156:THR:HG22	1:D:157:ASP:H	1.54	0.71
1:A:101:PRO:HG2	1:A:104:ASP:HB2	1.73	0.70
1:B:166:ALA:HB3	1:B:192:TRP:CZ3	2.27	0.69
1:C:94:GLY:HA3	1:C:285:VAL:HG23	1.73	0.69
1:B:94:GLY:HA3	1:B:285:VAL:CG2	2.22	0.69
1:G:159:ILE:HD13	1:G:199:PRO:HG2	1.75	0.69
1:B:94:GLY:HA3	1:B:285:VAL:HG23	1.74	0.68
1:C:166:ALA:HB3	1:C:192:TRP:CZ3	2.27	0.68
1:D:126:LEU:N	1:D:126:LEU:HD23	2.09	0.68
1:E:94:GLY:HA3	1:E:285:VAL:HG23	1.75	0.68
1:E:159:ILE:HD13	1:E:199:PRO:HG2	1.75	0.67
1:F:109:ARG:HD3	1:F:235:THR:HG21	1.75	0.67
1:A:170:ASP:OD2	1:A:172:LYS:HD2	1.96	0.66
1:B:86:THR:N	1:B:289:GLY:O	2.28	0.66
1:C:88:ILE:HG12	1:C:257:GLN:HG2	1.77	0.66
1:B:165:ASN:O	1:B:166:ALA:HB2	1.95	0.65
1:E:94:GLY:HA3	1:E:285:VAL:CG2	2.26	0.65
1:H:94:GLY:HA3	1:H:285:VAL:CG2	2.27	0.65
1:F:88:ILE:HG12	1:F:257:GLN:HG2	1.79	0.65
1:D:166:ALA:CB	1:D:192:TRP:CZ3	2.78	0.65
1:F:94:GLY:HA3	1:F:285:VAL:CG2	2.26	0.64
1:G:94:GLY:HA3	1:G:285:VAL:CG2	2.28	0.64
1:F:120:VAL:HA	1:F:169:ASN:O	1.98	0.63
1:D:156:THR:HG22	1:D:157:ASP:N	2.13	0.63
1:H:162:GLU:HG2	1:H:164:SER:OG	1.98	0.63
1:H:88:ILE:HG12	1:H:257:GLN:HG2	1.81	0.62
1:C:94:GLY:HA3	1:C:285:VAL:CG2	2.29	0.62
1:D:88:ILE:HG12	1:D:257:GLN:HG2	1.80	0.62
1:F:166:ALA:CB	1:F:192:TRP:CZ3	2.82	0.62
1:E:88:ILE:HG12	1:E:257:GLN:HG2	1.82	0.62
1:F:109:ARG:HD3	1:F:235:THR:CG2	2.30	0.62
1:D:148:ILE:HG22	2:D:4045:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ASP:OD1	1:F:172:LYS:HB2	1.99	0.61
1:B:88:ILE:HG12	1:B:257:GLN:HG2	1.81	0.61
1:B:166:ALA:HB1	1:B:192:TRP:CH2	2.36	0.61
1:E:89:PHE:CE1	1:E:258:LEU:HD12	2.35	0.61
1:H:82:HIS:HA	1:H:173:TYR:CE1	2.35	0.61
1:A:94:GLY:HA3	1:A:285:VAL:CG2	2.29	0.61
1:D:109:ARG:HD3	1:D:235:THR:CG2	2.30	0.61
1:F:166:ALA:HB3	1:F:192:TRP:CZ3	2.36	0.60
1:D:266:LEU:HB3	1:D:271:MET:CE	2.27	0.60
1:C:266:LEU:HB3	1:C:271:MET:CE	2.28	0.60
1:C:275:ASN:HD22	1:C:275:ASN:N	2.01	0.59
1:E:102:PRO:HG3	1:F:103:ASN:ND2	2.18	0.59
1:C:120:VAL:C	1:C:169:ASN:HD21	2.10	0.59
1:D:126:LEU:HD22	1:D:254:PHE:CD1	2.38	0.59
1:A:88:ILE:HG12	1:A:257:GLN:HG2	1.85	0.59
1:D:103:ASN:N	1:D:103:ASN:ND2	2.51	0.58
1:E:139:LEU:HD13	1:E:152:PHE:HB3	1.85	0.58
1:H:287:LEU:HD12	1:H:288:VAL:H	1.69	0.58
1:B:126:LEU:HD22	1:B:254:PHE:CD1	2.40	0.57
1:B:266:LEU:HB3	1:B:271:MET:CE	2.32	0.57
1:C:184:ASN:OD1	1:C:198:TYR:HA	2.04	0.57
1:H:99:LYS:HG2	1:H:242:THR:HG22	1.85	0.57
1:G:139:LEU:HD12	1:G:139:LEU:C	2.31	0.56
1:E:156:THR:HB	1:E:233:GLN:OE1	2.05	0.56
1:H:117:PHE:CZ	1:H:168:ILE:HD13	2.40	0.56
1:F:109:ARG:CD	1:F:235:THR:CG2	2.84	0.56
1:F:166:ALA:O	1:F:167:ILE:HG23	2.06	0.55
1:H:167:ILE:HD12	1:H:167:ILE:C	2.32	0.55
1:H:123:GLU:O	1:H:124:ALA:HB2	2.06	0.55
1:E:291:VAL:CG1	1:E:292:PRO:CD	2.84	0.54
1:E:147:LYS:HD2	1:E:164:SER:HA	1.89	0.54
1:G:156:THR:HB	1:G:233:GLN:OE1	2.06	0.54
1:E:126:LEU:HD22	1:E:254:PHE:CD1	2.42	0.53
1:E:266:LEU:HB3	1:E:271:MET:CE	2.34	0.53
1:F:120:VAL:C	1:F:169:ASN:HD21	2.16	0.53
1:D:123:GLU:O	1:D:124:ALA:HB2	2.09	0.53
1:A:162:GLU:OE2	1:A:164:SER:HB3	2.08	0.52
1:G:99:LYS:HG2	1:G:242:THR:HG22	1.90	0.52
1:E:139:LEU:CD1	1:E:152:PHE:HB3	2.39	0.52
1:E:160:ALA:O	1:E:197:ARG:HD3	2.10	0.52
1:A:160:ALA:O	1:A:197:ARG:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ARG:CD	1:F:235:THR:HG21	2.39	0.51
1:A:266:LEU:HB3	1:A:271:MET:CE	2.36	0.51
1:E:291:VAL:HG13	1:E:292:PRO:CD	2.38	0.51
1:A:126:LEU:HD13	1:A:258:LEU:HD21	1.92	0.50
1:G:126:LEU:HD22	1:G:254:PHE:CD1	2.46	0.50
1:G:101:PRO:HG2	1:G:104:ASP:OD2	2.12	0.50
1:H:156:THR:OG1	1:H:157:ASP:N	2.41	0.50
1:A:99:LYS:HG2	1:A:242:THR:HG22	1.94	0.50
1:E:192:TRP:CD1	1:E:192:TRP:N	2.79	0.49
1:G:160:ALA:O	1:G:197:ARG:HD3	2.12	0.49
1:B:85:THR:OG1	1:B:270:ASN:ND2	2.46	0.49
1:F:192:TRP:N	1:F:192:TRP:CD1	2.78	0.49
1:A:288:VAL:HG12	1:A:289:GLY:O	2.13	0.49
1:F:88:ILE:HG13	1:F:288:VAL:HG23	1.93	0.49
1:H:109:ARG:HG2	1:H:235:THR:CG2	2.33	0.49
1:A:163:GLU:HA	1:A:195:ILE:CD1	2.43	0.48
1:A:161:ILE:HD12	1:A:197:ARG:HB3	1.95	0.48
1:A:123:GLU:O	1:A:124:ALA:HB2	2.14	0.48
1:A:126:LEU:HD22	1:A:254:PHE:CD1	2.49	0.48
1:F:266:LEU:HB3	1:F:271:MET:CE	2.37	0.48
1:G:183:GLY:O	1:G:199:PRO:HG2	2.14	0.48
1:B:123:GLU:O	1:B:124:ALA:HB2	2.13	0.48
1:C:120:VAL:C	1:C:169:ASN:ND2	2.71	0.48
1:C:162:GLU:HG2	1:C:164:SER:OG	2.14	0.48
1:D:84:GLY:O	1:D:85:THR:C	2.57	0.47
1:H:117:PHE:HE1	1:H:168:ILE:HD13	1.76	0.47
1:D:146:GLY:O	1:D:167:ILE:HA	2.14	0.47
1:D:165:ASN:O	1:D:166:ALA:HB2	2.13	0.47
1:C:261:LEU:HD23	1:C:268:VAL:HB	1.95	0.47
1:D:192:TRP:CD1	1:D:192:TRP:N	2.81	0.47
1:F:120:VAL:C	1:F:169:ASN:ND2	2.73	0.47
1:G:81:GLY:HA3	1:G:173:TYR:CE2	2.49	0.47
1:A:157:ASP:OD2	1:F:197:ARG:NH1	2.48	0.47
1:C:270:ASN:O	1:C:274:GLU:HG3	2.14	0.47
1:F:85:THR:OG1	1:F:270:ASN:ND2	2.48	0.47
1:F:261:LEU:HD23	1:F:268:VAL:HB	1.98	0.46
1:A:192:TRP:CD1	1:A:192:TRP:N	2.82	0.46
1:E:101:PRO:O	1:E:102:PRO:C	2.59	0.46
1:F:166:ALA:C	1:F:167:ILE:HG12	2.39	0.46
1:E:163:GLU:OE2	1:E:165:ASN:HB2	2.15	0.46
1:G:117:PHE:HA	1:G:257:GLN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:LEU:HB3	1:H:271:MET:CE	2.40	0.46
1:C:117:PHE:HA	1:C:257:GLN:O	2.16	0.46
1:H:84:GLY:O	1:H:85:THR:C	2.59	0.46
1:C:123:GLU:O	1:C:124:ALA:HB2	2.15	0.46
1:C:192:TRP:CD1	1:C:192:TRP:N	2.83	0.46
1:G:90:SER:O	1:G:91:LYS:C	2.58	0.46
1:B:126:LEU:HD13	1:B:258:LEU:HD21	1.98	0.46
1:A:122:LYS:O	1:A:143:ILE:HG22	2.16	0.46
1:A:192:TRP:CB	1:A:193:PRO:HD2	2.31	0.46
1:B:274:GLU:OE2	1:G:109:ARG:NH2	2.47	0.45
1:C:148:ILE:HG22	2:C:4051:HOH:O	2.15	0.45
1:A:192:TRP:HB3	1:A:193:PRO:CD	2.34	0.45
1:B:126:LEU:N	1:B:126:LEU:HD23	2.31	0.45
1:C:156:THR:CB	1:C:233:GLN:HG3	2.28	0.45
1:G:268:VAL:CA	1:G:271:MET:HE3	2.41	0.45
1:A:167:ILE:HG23	1:A:169:ASN:OD1	2.17	0.45
1:A:159:ILE:HD13	1:A:199:PRO:HG3	1.97	0.45
1:G:162:GLU:HG2	1:G:164:SER:OG	2.17	0.45
1:C:126:LEU:HD13	1:C:258:LEU:HD21	1.99	0.45
1:A:90:SER:O	1:A:91:LYS:C	2.59	0.44
1:C:90:SER:O	1:C:91:LYS:C	2.60	0.44
1:G:88:ILE:HG12	1:G:257:GLN:CG	2.45	0.44
1:F:238:ASN:O	1:F:239:SER:C	2.60	0.44
1:G:122:LYS:O	1:G:143:ILE:HG22	2.18	0.44
1:C:159:ILE:HD13	1:C:199:PRO:HG2	1.98	0.44
1:F:137:ASP:HB3	1:F:237:PHE:CD1	2.52	0.44
1:D:143:ILE:HA	1:D:147:LYS:O	2.18	0.44
1:G:137:ASP:HA	1:G:153:ASN:O	2.18	0.44
1:A:120:VAL:HA	1:A:169:ASN:O	2.17	0.43
1:H:192:TRP:N	1:H:192:TRP:CD1	2.84	0.43
1:F:109:ARG:HG2	1:F:235:THR:CG2	2.49	0.43
1:A:101:PRO:HA	1:A:102:PRO:HD3	1.84	0.43
1:F:125:VAL:HG22	1:F:142:HIS:HB3	2.00	0.43
1:F:155:GLY:HA3	1:F:234:LEU:HD12	2.01	0.43
1:B:288:VAL:C	1:G:236:ILE:HD11	2.44	0.43
1:E:196:GLU:HB3	1:E:198:TYR:HE1	1.84	0.43
1:G:189:VAL:O	1:G:190:ASP:C	2.62	0.43
1:C:275:ASN:N	1:C:275:ASN:ND2	2.65	0.43
1:G:168:ILE:HD12	1:G:168:ILE:C	2.44	0.43
1:F:99:LYS:O	1:F:278:ASN:HB3	2.18	0.43
1:H:89:PHE:CE1	1:H:258:LEU:HD12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ILE:HD11	1:E:233:GLN:HG3	2.01	0.43
1:B:167:ILE:HD12	1:B:167:ILE:HA	1.86	0.42
1:D:166:ALA:HB1	1:D:192:TRP:CH2	2.54	0.42
1:H:172:LYS:HG2	1:H:173:TYR:N	2.34	0.42
1:D:167:ILE:N	1:D:167:ILE:HD13	2.35	0.42
1:D:288:VAL:CG1	1:D:289:GLY:N	2.82	0.42
1:G:88:ILE:HG21	1:G:88:ILE:HD13	1.79	0.42
1:E:137:ASP:HA	1:E:153:ASN:O	2.19	0.42
1:D:287:LEU:HG	1:E:236:ILE:HD13	2.00	0.42
1:A:276:ASP:OD1	1:A:277:ALA:N	2.53	0.42
1:B:88:ILE:HD12	1:H:234:LEU:HD11	2.00	0.42
1:H:261:LEU:HD23	1:H:268:VAL:HB	2.01	0.42
1:B:82:HIS:HA	1:B:173:TYR:CE1	2.55	0.41
1:C:99:LYS:HG2	1:C:242:THR:HG22	2.02	0.41
1:D:126:LEU:N	1:D:126:LEU:CD2	2.82	0.41
1:E:170:ASP:OD1	1:E:170:ASP:N	2.53	0.41
1:B:168:ILE:C	1:B:168:ILE:HD12	2.46	0.41
1:E:90:SER:O	1:E:91:LYS:C	2.63	0.41
1:E:159:ILE:HD13	1:E:199:PRO:CG	2.49	0.41
1:G:192:TRP:CD1	1:G:192:TRP:N	2.88	0.41
1:F:166:ALA:HB3	1:F:192:TRP:HZ3	1.81	0.41
1:H:235:THR:HG22	1:H:236:ILE:HG13	2.03	0.41
1:B:261:LEU:HB3	1:B:269:LEU:HG	2.03	0.41
1:D:156:THR:CG2	1:D:157:ASP:H	2.21	0.41
1:A:117:PHE:HA	1:A:257:GLN:O	2.20	0.41
1:E:196:GLU:HB3	1:E:198:TYR:CE1	2.56	0.41
1:H:169:ASN:O	1:H:169:ASN:CG	2.63	0.41
1:G:184:ASN:OD1	1:G:199:PRO:HD2	2.21	0.41
1:A:99:LYS:O	1:A:278:ASN:HB3	2.21	0.40
1:E:268:VAL:CA	1:E:271:MET:HE3	2.46	0.40
1:B:189:VAL:O	1:B:190:ASP:C	2.62	0.40
1:D:155:GLY:HA3	1:D:234:LEU:HD12	2.03	0.40
1:C:167:ILE:C	1:C:167:ILE:HD12	2.46	0.40
1:B:101:PRO:HA	1:B:102:PRO:HD3	1.87	0.40
1:G:159:ILE:HD13	1:G:199:PRO:CG	2.48	0.40
1:B:84:GLY:O	1:B:85:THR:C	2.63	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	A	178/182 (98%)	165 (93%)	13 (7%)	0	100	100
1	B	176/182 (97%)	164 (93%)	11 (6%)	1 (1%)	21	42
1	C	178/182 (98%)	168 (94%)	9 (5%)	1 (1%)	21	42
1	D	176/182 (97%)	162 (92%)	12 (7%)	2 (1%)	11	25
1	E	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	11	25
1	F	175/182 (96%)	162 (93%)	10 (6%)	3 (2%)	7	15
1	G	180/182 (99%)	168 (93%)	11 (6%)	1 (1%)	21	42
1	H	175/182 (96%)	161 (92%)	13 (7%)	1 (1%)	21	42
All	All	1417/1456 (97%)	1318 (93%)	88 (6%)	11 (1%)	16	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	156	THR
1	G	85	THR
1	B	166	ALA
1	E	83	ALA
1	F	102	PRO
1	F	165	ASN
1	F	170	ASP
1	H	124	ALA
1	D	124	ALA
1	E	91	LYS
1	C	91	LYS

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	145/146 (99%)	137 (94%)	8 (6%)	19	41
1	B	143/146 (98%)	135 (94%)	8 (6%)	19	40
1	C	145/146 (99%)	134 (92%)	11 (8%)	12	27
1	D	143/146 (98%)	133 (93%)	10 (7%)	14	31
1	E	146/146 (100%)	137 (94%)	9 (6%)	16	36
1	F	143/146 (98%)	132 (92%)	11 (8%)	12	27
1	G	146/146 (100%)	136 (93%)	10 (7%)	14	32
1	H	143/146 (98%)	136 (95%)	7 (5%)	22	47
All	All	1154/1168 (99%)	1080 (94%)	74 (6%)	16	35

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	162	GLU
1	A	167	ILE
1	A	179	THR
1	A	186	THR
1	A	197	ARG
1	A	279	ILE
1	A	291	VAL
1	B	126	LEU
1	B	162	GLU
1	B	167	ILE
1	B	179	THR
1	B	186	THR
1	B	199	PRO
1	B	279	ILE
1	B	282	VAL
1	C	104	ASP
1	C	126	LEU
1	C	139	LEU
1	C	162	GLU
1	C	168	ILE
1	C	169	ASN
1	C	179	THR
1	C	186	THR

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Mol	Chain	Res	Type
1	C	197	ARG
1	C	233	GLN
1	C	275	ASN
1	D	103	ASN
1	D	126	LEU
1	D	139	LEU
1	D	162	GLU
1	D	167	ILE
1	D	168	ILE
1	D	179	THR
1	D	186	THR
1	D	235	THR
1	D	279	ILE
1	E	101	PRO
1	E	126	LEU
1	E	162	GLU
1	E	179	THR
1	E	181	SER
1	E	186	THR
1	E	197	ARG
1	E	235	THR
1	E	275	ASN
1	F	90	SER
1	F	126	LEU
1	F	139	LEU
1	F	156	THR
1	F	162	GLU
1	F	167	ILE
1	F	179	THR
1	F	186	THR
1	F	235	THR
1	F	279	ILE
1	F	282	VAL
1	G	82	HIS
1	G	126	LEU
1	G	139	LEU
1	G	162	GLU
1	G	179	THR
1	G	186	THR
1	G	197	ARG
1	G	279	ILE
1	G	290	GLU

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Mol	Chain	Res	Type
1	G	291	VAL
1	H	99	LYS
1	H	126	LEU
1	H	162	GLU
1	H	179	THR
1	H	186	THR
1	H	235	THR
1	H	282	VAL

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	238	ASN
1	A	270	ASN
1	B	169	ASN
1	B	257	GLN
1	B	270	ASN
1	C	169	ASN
1	C	233	GLN
1	C	257	GLN
1	C	270	ASN
1	C	275	ASN
1	C	284	ASN
1	D	103	ASN
1	D	238	ASN
1	D	257	GLN
1	D	270	ASN
1	E	238	ASN
1	E	257	GLN
1	E	270	ASN
1	F	238	ASN
1	F	270	ASN
1	G	238	ASN
1	G	252	GLN
1	G	270	ASN
1	H	270	ASN
1	H	278	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.