



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:34 AM UTC

PDB ID : 3HHR / pdb_00003hhr
Title : HUMAN GROWTH HORMONE AND EXTRACELLULAR DOMAIN OF ITS RECEPTOR: CRYSTAL STRUCTURE OF THE COMPLEX
Authors : De Vos, A.M.; Ultsch, M.; Kossiakoff, A.A.
Deposited on : 1993-12-30
Resolution : 2.80 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

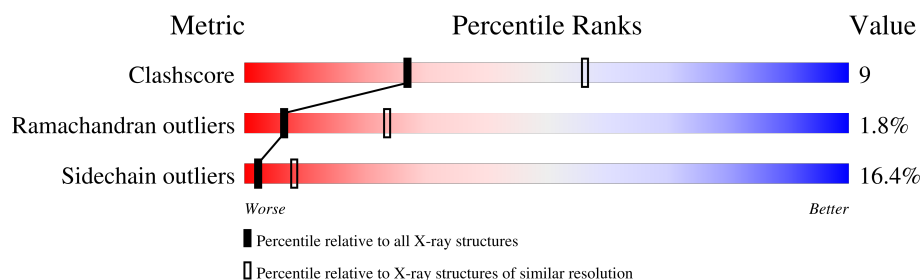
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	190	
2	B	205	
2	C	205	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4614 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 HUMAN GROWTH HORMONE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	1
			1479	943	249	280	7			

- Molecule 2 is a protein called HUMAN GROWTH HORMONE RECEPTOR (hGHbp).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	2
			1585	1014	261	301	9			
2	C	196	Total	C	N	O	S	0	0	2
			1550	992	253	295	10			

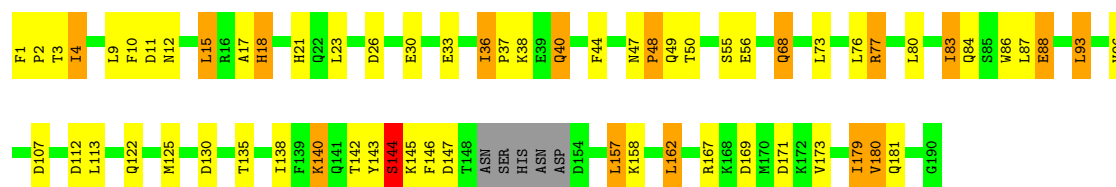
3 Residue-property plots

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.

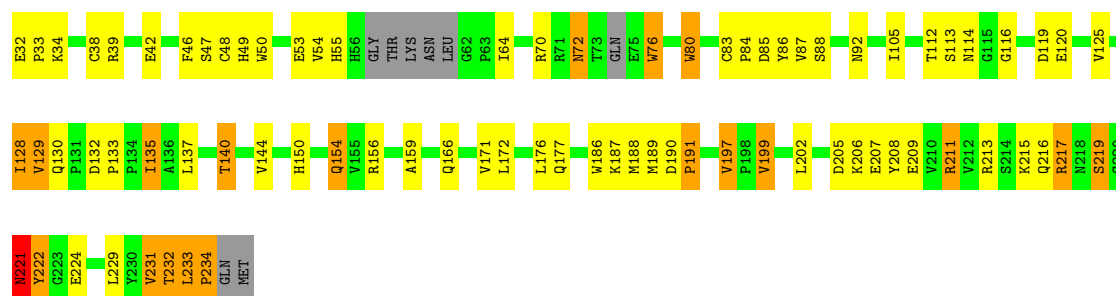
• Molecule 1: HUMAN GROWTH HORMONE

Chain A: 



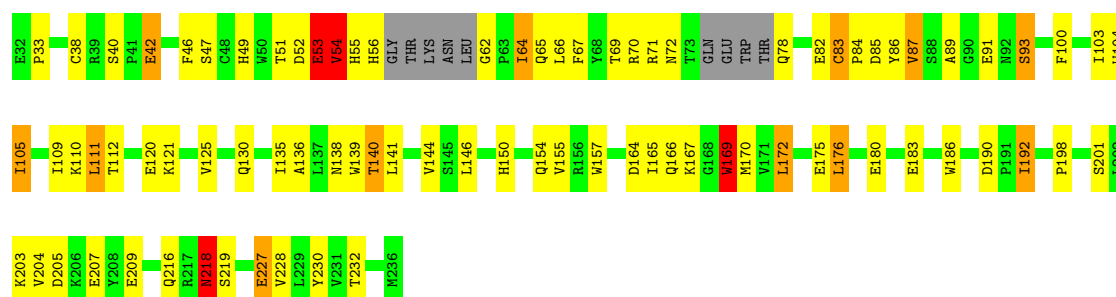
• Molecule 2: HUMAN GROWTH HORMONE RECEPTOR (hGHbp)

Chain B: 



• Molecule 2: HUMAN GROWTH HORMONE RECEPTOR (hGHbp)

Chain C: 



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	145.80Å 68.60Å 76.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.221 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.93	2/1509 (0.1%)	1.79	32/2037 (1.6%)
2	B	1.05	8/1629 (0.5%)	1.82	30/2219 (1.4%)
2	C	1.03	5/1592 (0.3%)	1.81	34/2169 (1.6%)
All	All	1.01	15/4730 (0.3%)	1.81	96/6425 (1.5%)

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
2	B	0	1
2	C	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	55	HIS	C-N	-7.08	1.23	1.33
2	B	72	ASN	C-N	-7.07	1.23	1.33
1	A	21	HIS	CD2-NE2	-7.01	1.30	1.37
2	C	150	HIS	CD2-NE2	-6.88	1.30	1.37
2	C	72	ASN	C-N	-6.71	1.24	1.33
2	B	150	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	147	ASP	C-N	-6.34	1.24	1.33
2	B	55	HIS	C-N	-6.30	1.24	1.33
2	B	133	PRO	CA-CB	-6.14	1.48	1.54
2	B	199	VAL	CA-CB	5.90	1.62	1.54
2	C	49	HIS	CD2-NE2	-5.80	1.31	1.37
2	B	105	ILE	CA-CB	5.59	1.58	1.54
2	B	128	ILE	CA-CB	5.55	1.61	1.54
2	B	49	HIS	CD2-NE2	-5.42	1.31	1.37
2	C	150	HIS	CG-ND1	-5.36	1.32	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	THR	N-CA-C	10.46	126.63	108.75
1	A	47	ASN	CA-CB-CG	9.92	122.52	112.60
1	A	144	SER	N-CA-C	9.50	131.04	110.80
1	A	3	THR	CA-C-N	-9.16	115.99	122.59
1	A	3	THR	C-N-CA	-9.16	115.99	122.59
2	C	85	ASP	CA-CB-CG	9.04	121.64	112.60
2	B	221	ASN	CA-CB-CG	8.94	121.54	112.60
2	C	218	ASN	CA-CB-CG	8.59	121.19	112.60
2	B	205	ASP	CA-CB-CG	8.37	120.97	112.60
2	B	105	ILE	CA-C-O	-8.25	114.39	119.51
1	A	145	LYS	N-CA-C	7.76	127.33	110.80
2	B	132	ASP	CA-C-N	7.55	125.09	119.66
2	B	132	ASP	C-N-CA	7.55	125.09	119.66
2	B	46	PHE	CA-CB-CG	7.35	121.15	113.80
2	C	172	LEU	N-CA-C	7.28	121.26	110.48
1	A	17	ALA	O-C-N	7.11	129.66	122.12
1	A	171	ASP	CA-CB-CG	7.11	119.71	112.60
2	B	87	VAL	CB-CA-C	-7.03	102.83	112.04
2	B	234	PRO	N-CA-C	6.96	129.51	112.10
1	A	130	ASP	CA-CB-CG	6.93	119.53	112.60
2	C	169	TRP	N-CA-C	-6.76	96.41	110.80
1	A	140	LYS	N-CA-C	-6.68	98.32	109.07
1	A	107	ASP	CA-CB-CG	6.63	119.23	112.60
2	C	46	PHE	CA-CB-CG	6.59	120.39	113.80
2	C	87	VAL	N-CA-CB	-6.58	100.38	111.23
2	B	135	ILE	N-CA-CB	-6.57	100.39	111.23
2	C	136	ALA	N-CA-C	6.57	124.80	110.80
2	B	150	HIS	N-CA-C	6.54	119.56	108.90
1	A	21	HIS	CB-CG-CD2	-6.49	122.76	131.20
2	B	86	TYR	N-CA-C	6.39	120.33	112.54
2	C	125	VAL	N-CA-C	6.36	117.14	110.72
2	B	150	HIS	CB-CG-CD2	-6.35	122.95	131.20
2	B	189	MET	O-C-N	6.33	130.84	123.30
2	B	48	CYS	CA-CB-SG	-6.28	99.96	114.40
1	A	88	GLU	CA-C-N	6.27	125.95	119.56
1	A	88	GLU	C-N-CA	6.27	125.95	119.56
2	B	189	MET	CA-C-O	6.24	127.10	120.36
1	A	4	ILE	CA-C-O	6.21	122.82	119.15
1	A	112	ASP	CA-CB-CG	6.19	118.79	112.60
2	B	76	TRP	CG-CD2-CE3	6.17	140.06	133.90
2	C	165	ILE	N-CA-CB	-6.13	102.81	110.47
2	B	87	VAL	N-CA-C	6.11	116.75	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	186	TRP	CG-CD2-CE3	6.10	140.00	133.90
2	C	93	SER	N-CA-C	6.04	118.14	109.14
2	C	112	THR	CA-CB-OG1	-6.04	100.55	109.60
2	C	216	GLN	CB-CG-CD	6.03	122.84	112.60
2	B	76	TRP	CB-CG-CD1	-5.97	117.95	126.90
2	C	216	GLN	CA-CB-CG	5.96	126.03	114.10
2	C	104	TRP	CE2-CD2-CE3	5.92	124.72	118.80
2	B	129	VAL	CB-CA-C	-5.89	102.55	111.33
2	C	140	THR	CA-CB-OG1	-5.89	100.77	109.60
2	C	201	SER	N-CA-C	5.86	120.01	112.86
2	B	120	GLU	CB-CG-CD	5.82	122.50	112.60
1	A	143	TYR	CA-CB-CG	5.81	124.36	113.90
1	A	179	ILE	CA-C-O	-5.78	114.94	120.95
2	C	150	HIS	CB-CG-CD2	-5.77	123.70	131.20
2	B	129	VAL	N-CA-CB	5.74	117.38	110.31
2	C	150	HIS	CA-CB-CG	5.58	119.38	113.80
2	C	83	CYS	CA-C-N	5.58	125.24	119.05
2	C	83	CYS	C-N-CA	5.58	125.24	119.05
2	B	85	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	158	LYS	O-C-N	5.56	127.80	122.07
1	A	18	HIS	O-C-N	-5.52	115.86	122.15
1	A	36	ILE	CA-C-N	5.50	125.48	120.03
1	A	36	ILE	C-N-CA	5.50	125.48	120.03
2	C	40	SER	CA-C-N	5.49	125.19	119.64
2	C	40	SER	C-N-CA	5.49	125.19	119.64
2	B	159	ALA	CA-C-N	5.47	125.47	119.90
2	B	159	ALA	C-N-CA	5.47	125.47	119.90
2	B	85	ASP	N-CA-C	5.44	117.56	107.60
2	C	83	CYS	N-CA-C	5.44	117.43	109.71
2	B	128	ILE	N-CA-CB	-5.43	105.10	112.22
1	A	17	ALA	CA-C-N	-5.41	112.61	120.29
1	A	17	ALA	C-N-CA	-5.41	112.61	120.29
2	C	53	GLU	CA-C-N	5.41	131.71	121.97
2	C	53	GLU	C-N-CA	5.41	131.71	121.97
2	C	49	HIS	CB-CG-CD2	-5.39	124.19	131.20
2	C	164	ASP	O-C-N	5.37	127.61	122.07
2	C	228	VAL	N-CA-CB	-5.36	104.69	110.53
1	A	142	THR	CA-C-N	-5.34	114.03	121.99
1	A	142	THR	C-N-CA	-5.34	114.03	121.99
1	A	4	ILE	N-CA-C	-5.34	102.37	107.76
2	B	88	SER	CA-C-O	-5.31	115.22	120.90
2	C	169	TRP	CE2-CD2-CG	-5.25	100.91	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	157	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	A	144	SER	N-CA-CB	-5.19	101.72	110.49
2	C	42	GLU	O-C-N	-5.16	115.87	122.94
1	A	86	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	26	ASP	N-CA-C	5.13	117.53	111.33
2	C	227	GLU	N-CA-C	-5.10	102.74	110.28
2	B	80	TRP	CE2-CD2-CG	-5.08	101.10	107.20
2	C	140	THR	CA-CB-CG2	5.06	119.09	110.50
2	B	140	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	56	GLU	CB-CG-CD	5.03	121.15	112.60
2	B	186	TRP	CG-CD2-CE3	5.03	138.93	133.90
1	A	36	ILE	N-CA-C	5.02	112.97	107.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	233	LEU	Peptide
2	C	62	GLY	Peptide

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	1479	0	1431	24	0
2	B	1585	0	1499	35	0
2	C	1550	0	1444	27	0
All	All	4614	0	4374	83	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 9.

All (83) 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)
2:C:207:GLU:HG3	2:C:232:THR:HG22	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:HIS:HE1	2:B:217:ARG:HD2	1.52	0.74
2:B:177:GLN:HE21	2:B:188:MET:HG2	1.53	0.72
2:C:64:ILE:HG22	2:C:111:LEU:HD22	1.76	0.68
2:C:66:LEU:HB3	2:C:83:CYS:HB2	1.80	0.64
2:C:52:ASP:HA	2:C:56:HIS:N	2.13	0.63
2:B:176:LEU:HD13	2:B:197:VAL:HG11	1.78	0.63
1:A:18:HIS:CE1	2:B:217:ARG:HD2	2.32	0.63
1:A:10:PHE:CZ	1:A:180:VAL:HG23	2.34	0.62
1:A:44:PHE:CD1	1:A:50:THR:HB	2.34	0.61
2:B:219:SER:HB3	2:B:221:ASN:ND2	2.15	0.61
2:B:39:ARG:HG3	2:B:130:GLN:HB3	1.83	0.61
2:C:71:ARG:HH11	2:C:71:ARG:HA	1.64	0.61
2:C:180:GLU:HB3	2:C:183:GLU:HB2	1.83	0.60
2:B:207:GLU:HG3	2:B:232:THR:HG23	1.83	0.60
1:A:10:PHE:HZ	1:A:180:VAL:HG23	1.67	0.59
2:C:155:VAL:HG21	2:C:176:LEU:HD21	1.86	0.58
2:B:208:TYR:HB2	2:B:231:VAL:HG13	1.86	0.58
2:C:83:CYS:HB3	2:C:86:TYR:CZ	2.39	0.57
2:B:33:PRO:HG3	2:B:53:GLU:H	1.70	0.57
2:C:69:THR:HG21	2:C:78:GLN:NE2	2.19	0.57
2:B:64:ILE:HA	2:B:112:THR:O	2.07	0.55
2:B:177:GLN:NE2	2:B:188:MET:HG2	2.21	0.55
2:C:65:GLN:O	2:C:111:LEU:HD23	2.08	0.53
2:C:82:GLU:HG2	2:C:83:CYS:N	2.24	0.53
2:C:38:CYS:HA	2:C:47:SER:O	2.08	0.53
2:C:70:ARG:HD3	2:C:105:ILE:HD11	1.91	0.53
2:B:171:VAL:HG13	2:B:217:ARG:HB2	1.91	0.52
2:C:169:TRP:O	2:C:170:MET:HB2	2.11	0.51
2:B:213:ARG:HD2	2:B:222:TYR:HB3	1.92	0.51
2:B:125:VAL:HA	2:B:128:ILE:HG22	1.93	0.50
2:B:219:SER:HB3	2:B:221:ASN:HD21	1.76	0.50
2:B:154:GLN:HG2	2:B:156:ARG:CZ	2.41	0.50
1:A:84:GLN:HA	1:A:87:LEU:HD13	1.93	0.49
2:B:209:GLU:HA	2:B:229:LEU:O	2.12	0.49
1:A:1:PHE:HB2	1:A:2:PRO:HD2	1.94	0.49
2:B:137:LEU:HB3	2:B:229:LEU:HD12	1.94	0.49
2:B:54:VAL:HG11	2:B:113:SER:OG	2.12	0.49
2:C:209:GLU:HG2	2:C:230:TYR:CE1	2.48	0.49
2:C:82:GLU:HG2	2:C:83:CYS:H	1.79	0.48
2:C:67:PHE:O	2:C:109:ILE:HA	2.15	0.47
1:A:68:GLN:HE21	1:A:179:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:THR:HA	2:B:116:GLY:O	2.15	0.47
1:A:44:PHE:HA	1:A:50:THR:OG1	2.15	0.47
1:A:77:ARG:NH1	1:A:80:LEU:HD23	2.31	0.46
2:B:32:GLU:C	2:B:53:GLU:HB2	2.40	0.46
2:C:33:PRO:HA	2:C:51:THR:O	2.16	0.46
1:A:55:SER:HA	1:A:144:SER:CB	2.45	0.46
2:B:33:PRO:HG2	2:B:64:ILE:HG12	1.98	0.46
1:A:76:LEU:HD21	1:A:180:VAL:HG21	1.97	0.45
2:B:38:CYS:HA	2:B:47:SER:O	2.16	0.45
2:C:53:GLU:O	2:C:54:VAL:HB	2.17	0.45
2:B:154:GLN:HE21	2:B:156:ARG:NH2	2.14	0.45
2:B:215:LYS:HB2	2:B:222:TYR:CE1	2.52	0.44
1:A:12:ASN:HA	1:A:15:LEU:HD23	1.98	0.44
2:B:128:ILE:HD12	2:B:128:ILE:HA	1.78	0.44
2:C:67:PHE:HB2	2:C:110:LYS:HG2	1.99	0.44
1:A:83:ILE:HD11	1:A:173:VAL:HG11	2.00	0.43
2:C:89:ALA:HB3	2:C:93:SER:HB2	1.99	0.43
2:B:135:ILE:HD12	2:B:135:ILE:HA	1.83	0.43
2:C:139:TRP:HB3	2:C:155:VAL:HG12	2.00	0.43
2:B:50:TRP:O	2:B:92:ASN:HB3	2.19	0.43
1:A:77:ARG:HG2	1:A:125:MET:HE1	2.00	0.43
2:B:176:LEU:HD13	2:B:197:VAL:CG1	2.47	0.43
2:C:209:GLU:HG2	2:C:230:TYR:HE1	1.82	0.42
1:A:37:PRO:HG2	1:A:40:GLN:HB2	2.01	0.42
2:C:83:CYS:HA	2:C:84:PRO:HD3	1.74	0.42
1:A:36:ILE:HA	1:A:37:PRO:HD2	1.94	0.42
1:A:1:PHE:HB2	1:A:2:PRO:CD	2.50	0.41
1:A:93:LEU:HD11	1:A:162:LEU:HB3	2.02	0.41
1:A:40:GLN:HE21	1:A:157:LEU:HD21	1.85	0.41
2:B:33:PRO:N	2:B:53:GLU:HB2	2.35	0.41
2:B:211:ARG:HH11	2:B:211:ARG:HD2	1.76	0.41
2:C:70:ARG:NH2	2:C:100:PHE:HA	2.36	0.41
2:C:154:GLN:HA	2:C:198:PRO:HA	2.00	0.41
2:C:190:ASP:O	2:C:192:ILE:HG23	2.20	0.41
1:A:169:ASP:O	1:A:173:VAL:HG23	2.21	0.41
2:B:221:ASN:O	2:B:222:TYR:HB2	2.21	0.41
1:A:18:HIS:CE1	2:B:217:ARG:CD	3.02	0.41
1:A:38:LYS:HA	1:A:38:LYS:HD3	1.87	0.41
2:B:190:ASP:HA	2:B:191:PRO:HD3	1.69	0.40
1:A:68:GLN:NE2	1:A:179:ILE:HD12	2.36	0.40
2:B:83:CYS:HA	2:B:84:PRO:HD2	1.92	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	181/190 (95%)	165 (91%)	12 (7%)	4 (2%)	5	19
2	B	191/205 (93%)	167 (87%)	23 (12%)	1 (0%)	24	55
2	C	190/205 (93%)	160 (84%)	25 (13%)	5 (3%)	4	15
All	All	562/600 (94%)	492 (88%)	60 (11%)	10 (2%)	6	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
2	C	54	VAL
2	C	169	TRP
1	A	138	ILE
2	C	167	LYS
2	B	222	TYR
2	C	218	ASN
2	C	219	SER
1	A	48	PRO
1	A	146	PHE

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	161/175 (92%)	136 (84%)	25 (16%)	2	9
2	B	176/191 (92%)	146 (83%)	30 (17%)	2	7
2	C	168/191 (88%)	140 (83%)	28 (17%)	2	8
All	All	505/557 (91%)	422 (84%)	83 (16%)	2	8

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LEU
1	A	11	ASP
1	A	15	LEU
1	A	23	LEU
1	A	30	GLU
1	A	33	GLU
1	A	40	GLN
1	A	48	PRO
1	A	49	GLN
1	A	68	GLN
1	A	73	LEU
1	A	77	ARG
1	A	83	ILE
1	A	88	GLU
1	A	93	LEU
1	A	96	VAL
1	A	113	LEU
1	A	122	GLN
1	A	140	LYS
1	A	157	LEU
1	A	162	LEU
1	A	167	ARG
1	A	180	VAL
1	A	181	GLN
2	B	34	LYS
2	B	42	GLU
2	B	70	ARG
2	B	72	ASN
2	B	76	TRP
2	B	80	TRP
2	B	114	ASN
2	B	119	ASP
2	B	129	VAL

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Mol	Chain	Res	Type
2	B	140	THR
2	B	144	VAL
2	B	154	GLN
2	B	166	GLN
2	B	172	LEU
2	B	187	LYS
2	B	191	PRO
2	B	197	VAL
2	B	199	VAL
2	B	202	LEU
2	B	206	LYS
2	B	211	ARG
2	B	216	GLN
2	B	217	ARG
2	B	219	SER
2	B	221	ASN
2	B	224	GLU
2	B	231	VAL
2	B	232	THR
2	B	233	LEU
2	B	234	PRO
2	C	42	GLU
2	C	53	GLU
2	C	54	VAL
2	C	64	ILE
2	C	87	VAL
2	C	91	GLU
2	C	103	ILE
2	C	105	ILE
2	C	111	LEU
2	C	120	GLU
2	C	121	LYS
2	C	130	GLN
2	C	135	ILE
2	C	138	ASN
2	C	140	THR
2	C	141	LEU
2	C	144	VAL
2	C	146	LEU
2	C	166	GLN
2	C	172	LEU
2	C	175	GLU

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Mol	Chain	Res	Type
2	C	176	LEU
2	C	192	ILE
2	C	203	LYS
2	C	204	VAL
2	C	205	ASP
2	C	218	ASN
2	C	227	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	21	HIS
1	A	40	GLN
1	A	46	GLN
1	A	68	GLN
1	A	181	GLN
2	B	154	GLN
2	C	78	GLN
2	C	92	ASN
2	C	235	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.