



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 AM GMT

PDB ID : 3HHR  
Title : HUMAN GROWTH HORMONE AND EXTRACELLULAR DOMAIN OF ITS RECEPTOR: CRYSTAL STRUCTURE OF THE COMPLEX  
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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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

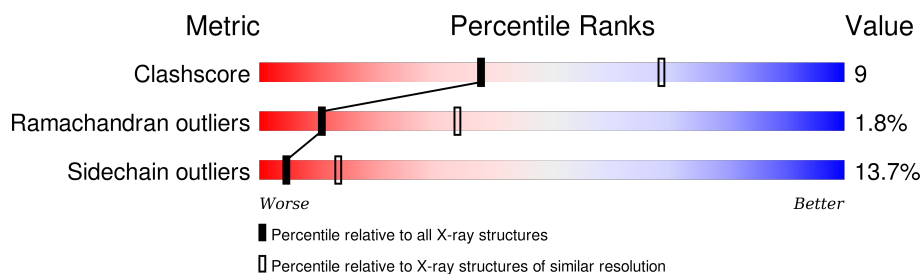
# 1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	190	 68% 23% 6% . .
2	B	205	 60% 29% 7% .
2	C	205	 59% 29% 6% . .

## 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).

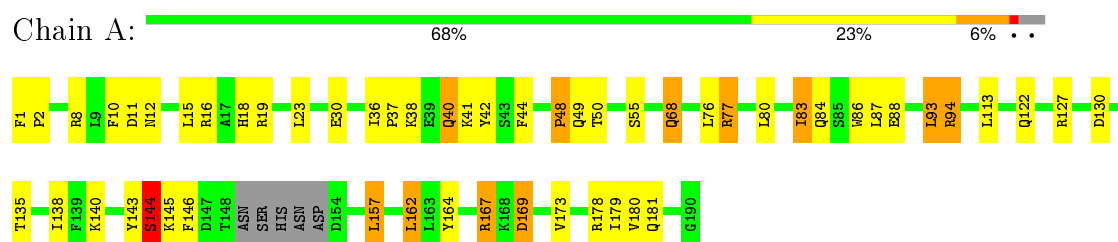
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	2
			1585	1014	261	301	9			
2	C	196	Total	C	N	O	S	0	0	2
			1550	992	253	295	10			

### 3 Residue-property plots [i](#)

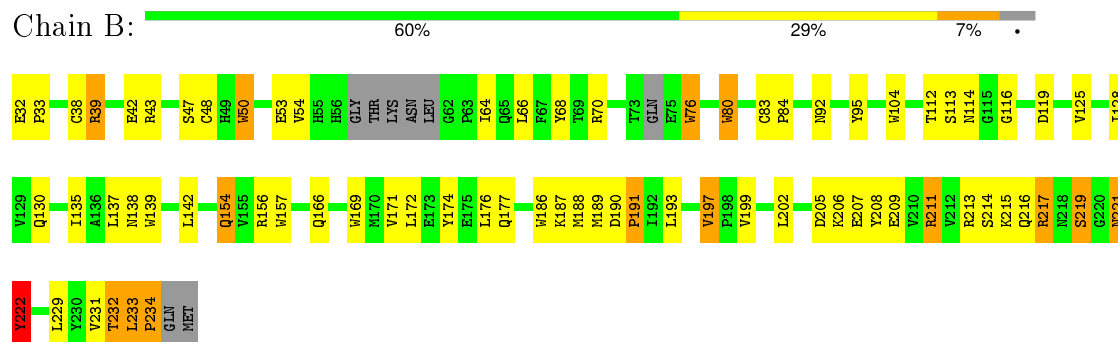
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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



#### • Molecule 2: HUMAN GROWTH HORMONE RECEPTOR (hGHbp)



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.80 Å 68.60 Å 76.00 Å 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 <sup>2</sup> )	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	0.74	0/1509	1.50	20/2037 (1.0%)
2	B	0.90	0/1629	1.65	39/2219 (1.8%)
2	C	0.88	0/1592	1.65	40/2169 (1.8%)
All	All	0.84	0/4730	1.60	99/6425 (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

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	169	TRP	CD1-CG-CD2	9.93	114.25	106.30
1	A	86	TRP	CD1-CG-CD2	9.48	113.88	106.30
1	A	42	TYR	CB-CG-CD2	-9.43	115.34	121.00
2	C	80	TRP	CD1-CG-CD2	9.15	113.62	106.30
2	C	50	TRP	CD1-CG-CD2	8.66	113.23	106.30
2	B	186	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	A	127	ARG	NE-CZ-NH2	-8.31	116.15	120.30
2	B	50	TRP	CD1-CG-CD2	8.22	112.88	106.30
2	B	139	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	A	178	ARG	NE-CZ-NH2	-8.05	116.27	120.30
2	C	186	TRP	CD1-CG-CD2	8.03	112.72	106.30
2	C	157	TRP	CD1-CG-CD2	8.02	112.71	106.30
2	C	169	TRP	CE2-CD2-CG	-7.99	100.91	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	86	TRP	CE2-CD2-CG	-7.85	101.02	107.30
2	C	176	LEU	CA-CB-CG	7.84	133.32	115.30
2	B	48	CYS	CA-CB-SG	-7.80	99.96	114.00
2	B	80	TRP	CE2-CD2-CG	-7.75	101.10	107.30
2	B	169	TRP	CD1-CG-CD2	7.69	112.45	106.30
2	B	76	TRP	CE2-CD2-CG	-7.46	101.33	107.30
2	C	80	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	144	SER	N-CA-C	7.42	131.04	111.00
2	B	50	TRP	CE2-CD2-CG	-7.37	101.41	107.30
2	C	157	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	B	157	TRP	CD1-CG-CD2	7.33	112.16	106.30
2	B	186	TRP	CE2-CD2-CG	-7.28	101.47	107.30
2	B	169	TRP	CE2-CD2-CG	-7.28	101.48	107.30
2	C	139	TRP	CD1-CG-CD2	7.24	112.09	106.30
2	C	186	TRP	CE2-CD2-CG	-7.17	101.56	107.30
2	C	50	TRP	CE2-CD2-CG	-7.03	101.67	107.30
2	B	139	TRP	CE2-CD2-CG	-6.98	101.71	107.30
2	B	76	TRP	CD1-CG-CD2	6.96	111.87	106.30
2	B	76	TRP	CB-CG-CD1	-6.96	117.95	127.00
2	B	189	MET	CA-C-N	-6.88	102.06	117.20
2	C	70	ARG	NE-CZ-NH1	6.87	123.74	120.30
2	B	76	TRP	CG-CD2-CE3	6.85	140.06	133.90
2	B	157	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	A	178	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	C	186	TRP	CG-CD2-CE3	6.78	140.00	133.90
2	C	139	TRP	CE2-CD2-CG	-6.73	101.92	107.30
2	B	234	PRO	N-CA-C	6.70	129.51	112.10
2	C	39	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	B	39	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	B	43	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	C	107	TYR	CB-CG-CD2	-6.24	117.25	121.00
2	B	104	TRP	CE2-CD2-CG	-6.24	102.31	107.30
2	C	169	TRP	CG-CD1-NE1	-6.20	103.90	110.10
1	A	19	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	C	43	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	B	104	TRP	CD1-CG-CD2	6.10	111.18	106.30
2	C	205	ASP	CA-C-N	-6.09	103.81	117.20
2	C	80	TRP	CG-CD1-NE1	-6.06	104.04	110.10
1	A	145	LYS	N-CA-C	6.05	127.33	111.00
1	A	16	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	86	TRP	CG-CD1-NE1	-5.95	104.15	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	144	SER	N-CA-CB	-5.86	101.72	110.50
2	C	186	TRP	CB-CG-CD1	-5.80	119.46	127.00
1	A	135	THR	N-CA-C	5.79	126.63	111.00
2	C	157	TRP	CG-CD2-CE3	5.78	139.10	133.90
2	C	48	CYS	CA-CB-SG	-5.77	103.61	114.00
1	A	143	TYR	CA-CB-CG	5.77	124.36	113.40
2	C	104	TRP	CE2-CD2-CG	-5.74	102.71	107.30
2	C	216	GLN	CA-CB-CG	5.74	126.03	113.40
2	B	50	TRP	CG-CD1-NE1	-5.71	104.39	110.10
2	B	193	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	8	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	94	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	C	50	TRP	CG-CD1-NE1	-5.61	104.49	110.10
2	B	66	LEU	CA-CB-CG	5.60	128.18	115.30
2	B	186	TRP	CG-CD2-CE3	5.59	138.93	133.90
2	B	222	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	C	169	TRP	CB-CG-CD1	-5.56	119.77	127.00
2	C	186	TRP	CG-CD1-NE1	-5.54	104.56	110.10
2	B	80	TRP	CB-CG-CD1	-5.48	119.87	127.00
2	C	104	TRP	CD1-CG-CD2	5.48	110.68	106.30
1	A	169	ASP	CB-CG-OD1	5.46	123.22	118.30
2	B	139	TRP	CG-CD1-NE1	-5.45	104.65	110.10
2	C	86	TYR	CB-CG-CD2	-5.41	117.75	121.00
2	C	169	TRP	N-CA-C	-5.41	96.41	111.00
2	C	157	TRP	CB-CG-CD1	-5.40	119.97	127.00
1	A	167	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	50	TRP	CG-CD2-CE3	5.39	138.75	133.90
2	B	186	TRP	CG-CD1-NE1	-5.34	104.76	110.10
2	B	68	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	C	169	TRP	CG-CD2-CE3	5.32	138.69	133.90
2	B	80	TRP	CG-CD2-CE3	5.27	138.65	133.90
2	C	157	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	B	233	LEU	CA-CB-CG	5.15	127.15	115.30
2	C	136	ALA	N-CA-C	5.11	124.80	111.00
2	C	66	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	164	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	B	189	MET	O-C-N	5.09	130.84	122.70
2	B	142	LEU	CA-CB-CG	5.08	126.98	115.30
2	C	87	VAL	N-CA-CB	-5.05	100.38	111.50
2	C	212	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	A	130	ASP	CB-CG-OD1	5.04	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	104	TRP	CE2-CD2-CE3	5.02	124.72	118.70
2	B	95	TYR	CB-CG-CD2	-5.00	118.00	121.00

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 [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	1479	0	1431	23	0
2	B	1585	0	1499	36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:69:THR:HG21	2:C:78:GLN:NE2	2.19	0.57
2:B:33:PRO:HG3	2:B:53:GLU:H	1.70	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:219:SER:HB3	2:B:221:ASN:HD21	1.76	0.50
2:B:125:VAL:HA	2:B:128:ILE:HG22	1.93	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
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: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:B:174:TYR:HE1	2:B:214:SER:HG	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:139:TRP:HB3	2:C:155:VAL:HG12	2.00	0.43
2:B:135:ILE:HD12	2:B:135:ILE:HA	1.83	0.43
2:B:50:TRP:O	2:B:92:ASN:HB3	2.19	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
2:B:32:GLU:C	2:B:53:GLU:HB2	2.40	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:C:70:ARG:NH2	2:C:100:PHE:HA	2.36	0.41
2:C:190:ASP:O	2:C:192:ILE:HG23	2.20	0.41
2:C:154:GLN:HA	2:C:198:PRO:HA	2.00	0.41
2:B:211:ARG:HH11	2:B:211:ARG:HD2	1.76	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 ⓘ

### 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	181/190 (95%)	165 (91%)	12 (7%)	4 (2%)	8	28
2	B	191/205 (93%)	167 (87%)	23 (12%)	1 (0%)	34	69
2	C	190/205 (93%)	160 (84%)	25 (13%)	5 (3%)	7	22
All	All	562/600 (94%)	492 (88%)	60 (11%)	10 (2%)	11	34

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 ⓘ

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%)	141 (88%)	20 (12%)	6	17
2	B	176/191 (92%)	152 (86%)	24 (14%)	5	14
2	C	168/191 (88%)	143 (85%)	25 (15%)	4	11
All	All	505/557 (91%)	436 (86%)	69 (14%)	4	13

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	23	LEU
1	A	30	GLU
1	A	40	GLN
1	A	41	LYS
1	A	48	PRO
1	A	49	GLN
1	A	68	GLN
1	A	77	ARG
1	A	83	ILE
1	A	88	GLU
1	A	93	LEU
1	A	94	ARG
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	181	GLN
2	B	42	GLU
2	B	70	ARG
2	B	76	TRP
2	B	80	TRP
2	B	114	ASN
2	B	119	ASP
2	B	138	ASN
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	205	ASP
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	232	THR

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Mol	Chain	Res	Type
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	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	141	LEU
2	C	144	VAL
2	C	146	LEU
2	C	166	GLN
2	C	172	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	69	GLN
2	B	92	ASN
2	B	130	GLN
2	B	138	ASN
2	B	154	GLN
2	C	78	GLN
2	C	92	ASN

### 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 carbohydrates 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 will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.