



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:14 PM UTC

PDB ID : 1HWH / pdb_00001hwh
Title : 1:1 COMPLEX OF HUMAN GROWTH HORMONE MUTANT G120R
WITH ITS SOLUBLE BINDING PROTEIN
Authors : Sundstrom, S.M.; Lundqvist, T.
Deposited on : 1996-11-13
Resolution : 2.90 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

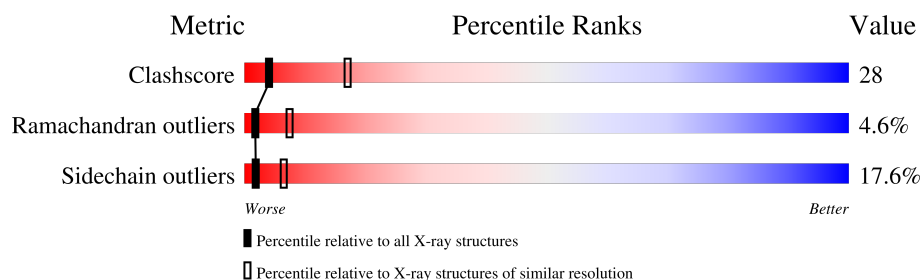
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	191	43% 39% 13% • •
2	B	237	34% 36% 11% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3034 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 GROWTH HORMONE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1474	940	246	281	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ARG	GLY	engineered mutation	UNP P01241

- Molecule 2 is a protein called GROWTH HORMONE BINDING PROTEIN.

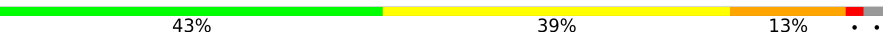
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1560	998	256	296	10			

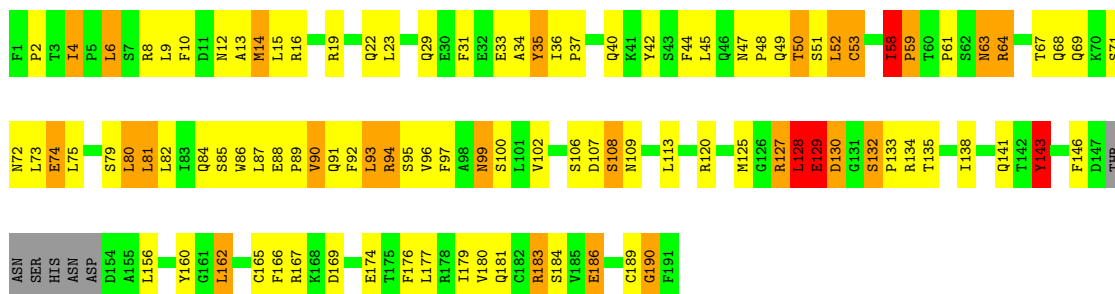
3 Residue-property plots

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.

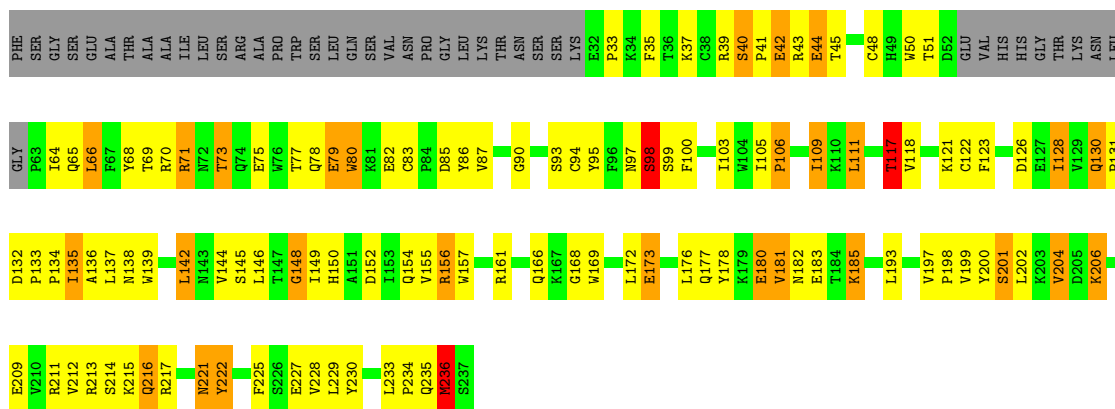
• Molecule 1: GROWTH HORMONE

Chain A: 



• Molecule 2: GROWTH HORMONE BINDING PROTEIN

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	67.78Å 67.78Å 229.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	91.8 (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.215 , 0.317	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3034	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	0.76	1/1503 (0.1%)	1.16	15/2033 (0.7%)
2	B	0.86	1/1603 (0.1%)	1.33	27/2186 (1.2%)
All	All	0.82	2/3106 (0.1%)	1.25	42/4219 (1.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	VAL	CA-CB	5.54	1.60	1.55
1	A	14	MET	SD-CE	5.21	1.92	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	THR	N-CA-C	-10.58	99.83	111.36
1	A	58	ILE	CA-C-N	8.70	130.71	119.84
1	A	58	ILE	C-N-CA	8.70	130.71	119.84
2	B	148	GLY	N-CA-C	-8.59	102.27	111.21
2	B	161	ARG	N-CA-C	7.71	121.79	112.38
2	B	79	GLU	N-CA-C	-7.63	102.34	112.72
2	B	73	THR	N-CA-C	7.17	126.07	110.80
1	A	13	ALA	N-CA-C	-7.14	102.69	111.40
2	B	87	VAL	N-CA-C	7.14	118.19	111.48
2	B	233	LEU	CA-C-N	7.08	126.60	119.24
2	B	233	LEU	C-N-CA	7.08	126.60	119.24
1	A	130	ASP	N-CA-C	6.76	120.28	108.52
1	A	166	PHE	N-CA-C	-6.49	103.11	111.02
2	B	75	GLU	N-CA-C	-6.47	100.38	109.69
2	B	168	GLY	N-CA-C	6.34	123.52	114.64
2	B	173	GLU	N-CA-C	-6.30	99.93	109.95
2	B	201	SER	N-CA-C	6.28	120.26	112.47
1	A	189	CYS	N-CA-C	-6.28	104.93	112.59
2	B	134	PRO	N-CA-C	-6.14	102.62	111.22
2	B	142	LEU	N-CA-C	-6.13	106.34	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	181	VAL	N-CA-C	6.07	119.55	111.17
2	B	130	GLN	CA-C-N	5.96	126.30	119.92
2	B	130	GLN	C-N-CA	5.96	126.30	119.92
2	B	117	THR	N-CA-C	-5.94	98.14	110.80
1	A	169	ASP	N-CA-C	5.67	117.54	111.36
2	B	145	SER	N-CA-C	5.62	122.76	110.80
2	B	227	GLU	N-CA-C	-5.56	102.66	110.50
1	A	15	LEU	N-CA-C	-5.54	104.06	112.04
2	B	90	GLY	N-CA-C	5.54	120.11	112.52
1	A	99	ASN	N-CA-C	-5.53	106.23	114.64
1	A	141	GLN	N-CA-C	5.53	118.25	109.24
2	B	37	LYS	N-CA-C	5.46	116.81	108.52
1	A	81	LEU	N-CA-C	5.43	116.88	111.07
1	A	190	GLY	N-CA-C	5.40	125.98	113.18
2	B	236	MET	N-CA-C	5.36	121.69	113.28
2	B	180	GLU	N-CA-C	-5.28	102.46	110.28
2	B	98	SER	N-CA-C	5.24	117.67	111.33
1	A	80	LEU	N-CA-C	-5.22	105.48	111.07
1	A	69	GLN	N-CA-C	-5.15	104.81	111.71
1	A	8	ARG	N-CA-C	-5.10	107.60	113.88
2	B	100	PHE	N-CA-C	-5.07	106.34	112.88
2	B	106	PRO	N-CA-C	5.04	119.11	111.19

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	1474	0	1425	81	0
2	B	1560	0	1453	82	0
All	All	3034	0	2878	161	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 28.

All (161) 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:A:73:LEU:HD23	1:A:132:SER:HB3	1.36	1.06
2:B:131:PRO:HD2	2:B:221:ASN:ND2	1.72	1.04
1:A:31:PHE:CE1	1:A:160:TYR:HB2	1.95	0.98
1:A:42:TYR:CD1	2:B:122:CYS:HB2	2.07	0.89
2:B:185:LYS:HD2	2:B:185:LYS:H	1.37	0.88
2:B:131:PRO:HD2	2:B:221:ASN:HD21	1.36	0.86
2:B:111:LEU:HD12	2:B:111:LEU:H	1.46	0.81
1:A:143:TYR:H	1:A:143:TYR:HD1	1.29	0.79
1:A:128:LEU:HD13	1:A:128:LEU:O	1.87	0.74
2:B:42:GLU:HG2	2:B:44:GLU:HB2	1.69	0.74
2:B:71:ARG:HG3	2:B:71:ARG:HH11	1.52	0.74
1:A:61:PRO:HD2	1:A:176:PHE:CZ	2.24	0.73
2:B:132:ASP:HB3	2:B:133:PRO:HD2	1.72	0.72
1:A:128:LEU:HD21	1:A:184:SER:HB2	1.71	0.72
2:B:95:TYR:HE1	2:B:97:ASN:HB3	1.53	0.72
2:B:185:LYS:H	2:B:185:LYS:CD	2.02	0.71
2:B:149:ILE:HG22	2:B:150:HIS:ND1	2.06	0.71
1:A:35:TYR:CB	1:A:156:LEU:HD11	2.20	0.70
1:A:86:TRP:O	1:A:90:VAL:HG22	1.91	0.70
2:B:221:ASN:ND2	2:B:222:TYR:N	2.41	0.69
2:B:103:ILE:HG23	2:B:126:ASP:HB3	1.75	0.69
1:A:6:LEU:HD12	1:A:6:LEU:H	1.60	0.67
2:B:138:ASN:HB2	2:B:156:ARG:HD2	1.76	0.66
2:B:139:TRP:HA	2:B:154:GLN:O	1.96	0.65
2:B:130:GLN:HA	2:B:221:ASN:ND2	2.12	0.65
1:A:71:SER:HB2	1:A:132:SER:HB2	1.80	0.65
1:A:53:CYS:HB3	1:A:165:CYS:SG	2.38	0.64
1:A:92:PHE:O	1:A:94:ARG:N	2.31	0.63
1:A:53:CYS:HG	1:A:165:CYS:HG	0.72	0.63
1:A:4:ILE:HG23	1:A:127:ARG:NH1	2.15	0.62
1:A:179:ILE:O	1:A:183:ARG:HG2	2.00	0.62
1:A:53:CYS:CB	1:A:165:CYS:SG	2.88	0.61
1:A:10:PHE:HB3	1:A:181:GLN:OE1	2.01	0.61
2:B:103:ILE:CG2	2:B:126:ASP:HB3	2.31	0.61
2:B:206:LYS:HB3	2:B:206:LYS:NZ	2.15	0.61
1:A:94:ARG:HA	1:A:107:ASP:HB3	1.82	0.60
2:B:42:GLU:CG	2:B:44:GLU:HB2	2.31	0.60
2:B:109:ILE:HG22	2:B:121:LYS:HB3	1.84	0.60
1:A:31:PHE:HE1	1:A:160:TYR:HB2	1.65	0.60
1:A:45:LEU:HA	1:A:51:SER:HB3	1.83	0.59
1:A:125:MET:O	1:A:129:GLU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:ILE:C	2:B:204:VAL:HG23	2.27	0.59
2:B:166:GLN:H	2:B:166:GLN:CD	2.12	0.58
2:B:149:ILE:O	2:B:204:VAL:HG23	2.04	0.57
2:B:236:MET:O	2:B:236:MET:HG2	2.04	0.57
1:A:53:CYS:CB	1:A:165:CYS:HG	2.15	0.57
1:A:35:TYR:O	1:A:36:ILE:HD13	2.04	0.56
2:B:111:LEU:HD13	2:B:118:VAL:HG23	1.89	0.55
2:B:149:ILE:HG22	2:B:150:HIS:CE1	2.42	0.55
2:B:137:LEU:HD12	2:B:229:LEU:HB2	1.89	0.55
2:B:215:LYS:HB2	2:B:222:TYR:CD1	2.42	0.54
1:A:186:GLU:H	1:A:186:GLU:CD	2.14	0.54
2:B:71:ARG:HG3	2:B:71:ARG:NH1	2.22	0.54
1:A:35:TYR:HB3	1:A:156:LEU:HD11	1.90	0.53
1:A:133:PRO:C	1:A:135:THR:H	2.16	0.53
1:A:72:ASN:OD1	1:A:180:VAL:HG13	2.09	0.53
1:A:94:ARG:CB	1:A:107:ASP:HB3	2.39	0.52
1:A:127:ARG:C	1:A:129:GLU:H	2.17	0.52
2:B:83:CYS:CB	2:B:94:CYS:SG	2.97	0.52
1:A:177:LEU:O	1:A:180:VAL:HB	2.09	0.52
1:A:35:TYR:CD1	1:A:35:TYR:N	2.77	0.52
1:A:94:ARG:CA	1:A:107:ASP:HB3	2.40	0.52
2:B:78:GLN:C	2:B:80:TRP:H	2.17	0.52
2:B:172:LEU:HD23	2:B:216:GLN:HA	1.91	0.52
1:A:34:ALA:HB3	1:A:35:TYR:CD1	2.45	0.52
1:A:95:SER:O	1:A:99:ASN:HB2	2.10	0.52
2:B:33:PRO:HG2	2:B:64:ILE:HD11	1.93	0.50
2:B:95:TYR:CE1	2:B:97:ASN:HB3	2.40	0.50
2:B:213:ARG:HD3	2:B:225:PHE:CE1	2.46	0.50
1:A:35:TYR:HB2	1:A:156:LEU:HD11	1.93	0.49
2:B:33:PRO:HG2	2:B:64:ILE:CD1	2.42	0.49
1:A:58:ILE:HD11	1:A:82:LEU:HD23	1.94	0.49
1:A:44:PHE:CZ	1:A:51:SER:HA	2.48	0.48
2:B:221:ASN:O	2:B:222:TYR:O	2.31	0.48
2:B:42:GLU:HG2	2:B:42:GLU:O	2.13	0.48
1:A:88:GLU:HB3	1:A:89:PRO:HD3	1.95	0.48
2:B:45:THR:HG22	2:B:98:SER:N	2.28	0.48
2:B:173:GLU:HG3	2:B:217:ARG:HG2	1.95	0.48
2:B:221:ASN:ND2	2:B:222:TYR:H	2.09	0.47
2:B:181:VAL:HG12	2:B:230:TYR:HE1	1.78	0.47
1:A:72:ASN:HD21	1:A:183:ARG:HD2	1.78	0.47
1:A:132:SER:HA	1:A:133:PRO:HD3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ILE:O	2:B:136:ALA:HB3	2.14	0.47
2:B:221:ASN:CG	2:B:222:TYR:N	2.72	0.47
2:B:50:TRP:CZ3	2:B:66:LEU:HD23	2.50	0.47
1:A:34:ALA:HB3	1:A:35:TYR:CE1	2.51	0.46
1:A:48:PRO:C	1:A:50:THR:H	2.23	0.46
1:A:9:LEU:HD12	1:A:9:LEU:H	1.81	0.46
1:A:80:LEU:O	1:A:84:GLN:HG3	2.15	0.46
1:A:97:PHE:HB3	1:A:106:SER:N	2.30	0.46
1:A:12:ASN:HB3	1:A:120:ARG:NH1	2.31	0.46
2:B:111:LEU:O	2:B:118:VAL:HG22	2.16	0.46
2:B:85:ASP:O	2:B:94:CYS:HA	2.16	0.46
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.74	0.45
2:B:138:ASN:HB2	2:B:156:ARG:CD	2.43	0.45
1:A:19:ARG:HD2	1:A:22:GLN:OE1	2.17	0.45
1:A:4:ILE:HD12	1:A:127:ARG:HH22	1.81	0.45
1:A:174:GLU:O	1:A:174:GLU:HG2	2.16	0.45
2:B:66:LEU:HA	2:B:111:LEU:HA	1.99	0.45
2:B:68:TYR:CD1	2:B:68:TYR:C	2.94	0.45
2:B:156:ARG:HG2	2:B:157:TRP:N	2.32	0.45
2:B:181:VAL:CG1	2:B:230:TYR:HE1	2.29	0.45
1:A:61:PRO:HB2	1:A:67:THR:OG1	2.17	0.45
2:B:214:SER:O	2:B:222:TYR:HA	2.17	0.45
1:A:85:SER:HA	1:A:143:TYR:HD2	1.81	0.45
1:A:93:LEU:HD21	1:A:162:LEU:HB3	1.98	0.45
2:B:221:ASN:CG	2:B:222:TYR:H	2.25	0.44
1:A:44:PHE:CD1	1:A:50:THR:HB	2.53	0.44
1:A:97:PHE:C	1:A:99:ASN:H	2.26	0.44
2:B:144:VAL:O	2:B:144:VAL:HG23	2.17	0.44
1:A:63:ASN:O	1:A:64:ARG:C	2.60	0.44
2:B:82:GLU:HG2	2:B:83:CYS:H	1.83	0.44
1:A:143:TYR:CD1	1:A:143:TYR:N	2.73	0.44
2:B:138:ASN:O	2:B:155:VAL:HA	2.17	0.44
2:B:212:VAL:HG12	2:B:213:ARG:N	2.33	0.43
1:A:52:LEU:HG	1:A:53:CYS:N	2.32	0.43
1:A:92:PHE:C	1:A:94:ARG:N	2.77	0.43
2:B:79:GLU:O	2:B:80:TRP:C	2.61	0.43
2:B:83:CYS:HB3	2:B:86:TYR:CZ	2.53	0.42
2:B:197:VAL:HG23	2:B:198:PRO:HD2	2.01	0.42
1:A:47:ASN:C	1:A:49:GLN:N	2.77	0.42
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.78	0.42
2:B:111:LEU:HD12	2:B:111:LEU:N	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:THR:O	2:B:117:THR:HG22	2.19	0.42
2:B:40:SER:HA	2:B:41:PRO:HD2	1.92	0.42
2:B:176:LEU:HD23	2:B:177:GLN:N	2.35	0.42
1:A:84:GLN:O	1:A:87:LEU:HB2	2.20	0.42
1:A:179:ILE:HD11	2:B:169:TRP:HE3	1.83	0.42
2:B:71:ARG:HB2	2:B:106:PRO:HG2	2.01	0.42
1:A:92:PHE:HE2	1:A:146:PHE:HD2	1.68	0.42
2:B:206:LYS:HB3	2:B:206:LYS:HZ2	1.82	0.42
1:A:37:PRO:HD2	1:A:40:GLN:HG3	2.02	0.42
1:A:72:ASN:O	1:A:73:LEU:C	2.62	0.42
1:A:74:GLU:O	1:A:75:LEU:C	2.60	0.42
1:A:88:GLU:O	1:A:91:GLN:HG3	2.19	0.42
2:B:82:GLU:HG2	2:B:83:CYS:N	2.34	0.42
1:A:128:LEU:O	1:A:130:ASP:N	2.53	0.41
1:A:58:ILE:HA	1:A:59:PRO:HD2	1.76	0.41
2:B:213:ARG:HB3	2:B:225:PHE:HA	2.01	0.41
1:A:88:GLU:O	1:A:89:PRO:C	2.61	0.41
1:A:95:SER:O	1:A:96:VAL:C	2.62	0.41
2:B:35:PHE:CE2	2:B:109:ILE:CG2	3.03	0.41
2:B:128:ILE:HD12	2:B:128:ILE:HA	1.85	0.41
2:B:209:GLU:HB2	2:B:228:VAL:CG2	2.50	0.41
2:B:152:ASP:OD2	2:B:200:TYR:HD1	2.03	0.41
1:A:92:PHE:CE2	1:A:146:PHE:HD2	2.39	0.41
2:B:69:THR:OG1	2:B:78:GLN:HA	2.20	0.41
2:B:123:PHE:C	2:B:123:PHE:CD1	2.98	0.41
2:B:48:CYS:O	2:B:93:SER:HA	2.21	0.41
2:B:148:GLY:O	2:B:149:ILE:HB	2.21	0.41
1:A:84:GLN:HA	1:A:87:LEU:HG	2.03	0.40
2:B:180:GLU:O	2:B:183:GLU:HG2	2.21	0.40
1:A:71:SER:O	1:A:72:ASN:C	2.63	0.40
1:A:100:SER:OG	1:A:102:VAL:HG23	2.21	0.40
1:A:14:MET:HE3	1:A:14:MET:HB3	1.80	0.40
1:A:22:GLN:O	1:A:22:GLN:HG2	2.21	0.40
2:B:149:ILE:HD13	2:B:149:ILE:HG21	1.91	0.40
2:B:178:TYR:HA	2:B:209:GLU:O	2.22	0.40
1:A:29:GLN:O	1:A:33:GLU:HG2	2.22	0.40
1:A:108:SER:O	1:A:109:ASN:C	2.65	0.40
2:B:166:GLN:CD	2:B:166:GLN:N	2.79	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	181/191 (95%)	134 (74%)	36 (20%)	11 (6%)	1	4
2	B	192/237 (81%)	161 (84%)	25 (13%)	6 (3%)	3	14
All	All	373/428 (87%)	295 (79%)	61 (16%)	17 (5%)	2	7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
2	B	73	THR
2	B	80	TRP
2	B	222	TYR
1	A	2	PRO
1	A	129	GLU
1	A	190	GLY
2	B	146	LEU
2	B	235	GLN
1	A	94	ARG
1	A	128	LEU
1	A	134	ARG
1	A	143	TYR
1	A	132	SER
1	A	59	PRO
2	B	117	THR
1	A	64	ARG

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	161/177 (91%)	136 (84%)	25 (16%)	2	9
2	B	168/217 (77%)	135 (80%)	33 (20%)	1	5
All	All	329/394 (84%)	271 (82%)	58 (18%)	2	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	LEU
1	A	16	ARG
1	A	23	LEU
1	A	35	TYR
1	A	50	THR
1	A	52	LEU
1	A	53	CYS
1	A	58	ILE
1	A	63	ASN
1	A	68	GLN
1	A	74	GLU
1	A	79	SER
1	A	90	VAL
1	A	108	SER
1	A	113	LEU
1	A	127	ARG
1	A	128	LEU
1	A	129	GLU
1	A	138	ILE
1	A	143	TYR
1	A	162	LEU
1	A	167	ARG
1	A	183	ARG
1	A	186	GLU
2	B	39	ARG
2	B	40	SER
2	B	42	GLU
2	B	43	ARG
2	B	44	GLU
2	B	51	THR
2	B	65	GLN
2	B	66	LEU
2	B	70	ARG

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Mol	Chain	Res	Type
2	B	71	ARG
2	B	98	SER
2	B	99	SER
2	B	105	ILE
2	B	109	ILE
2	B	111	LEU
2	B	117	THR
2	B	128	ILE
2	B	135	ILE
2	B	142	LEU
2	B	156	ARG
2	B	182	ASN
2	B	185	LYS
2	B	193	LEU
2	B	199	VAL
2	B	201	SER
2	B	202	LEU
2	B	204	VAL
2	B	206	LYS
2	B	211	ARG
2	B	216	GLN
2	B	221	ASN
2	B	234	PRO
2	B	236	MET

Sometimes 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	46	GLN
1	A	63	ASN
1	A	68	GLN
2	B	114	ASN
2	B	130	GLN
2	B	177	GLN
2	B	216	GLN
2	B	218	ASN
2	B	221	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 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.