



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 3NPZ / pdb_00003npz
Title : Prolactin Receptor (PRLR) Complexed with the Natural Hormone (PRL)
Authors : Van Agthoven, J.; England, P.; Goffin, V.; Broutin, I.
Deposited on : 2010-06-29
Resolution : 3.35 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

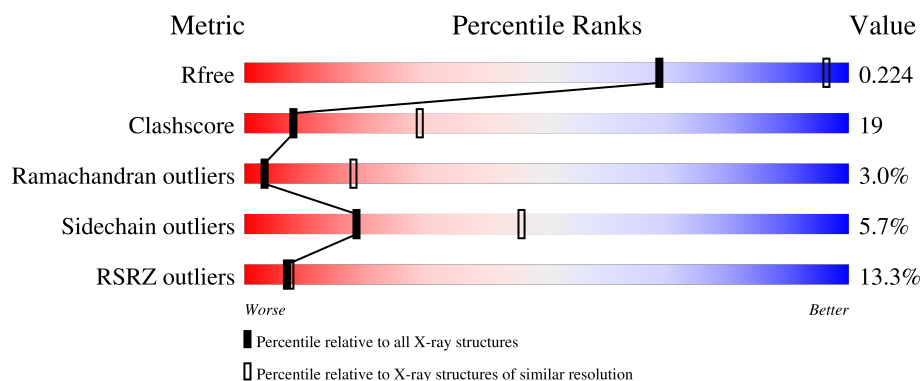
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	199	12% 52% 34% 7% 7%
2	B	220	8% 60% 29% • 8%
2	C	220	17% 52% 33% 5% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4817 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 Prolactin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1507	949	266	283	9			

- Molecule 2 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	202	Total	C	N	O	S	0	0	0
			1666	1072	267	319	8			
2	C	199	Total	C	N	O	S	0	0	0
			1644	1058	264	314	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ARG	-	expression tag	UNP P05710
B	212	SER	-	expression tag	UNP P05710
B	213	ARG	-	expression tag	UNP P05710
B	214	SER	-	expression tag	UNP P05710
B	215	HIS	-	expression tag	UNP P05710
B	216	HIS	-	expression tag	UNP P05710
B	217	HIS	-	expression tag	UNP P05710
B	218	HIS	-	expression tag	UNP P05710
B	219	HIS	-	expression tag	UNP P05710
B	220	HIS	-	expression tag	UNP P05710
C	211	ARG	-	expression tag	UNP P05710
C	212	SER	-	expression tag	UNP P05710
C	213	ARG	-	expression tag	UNP P05710
C	214	SER	-	expression tag	UNP P05710
C	215	HIS	-	expression tag	UNP P05710
C	216	HIS	-	expression tag	UNP P05710
C	217	HIS	-	expression tag	UNP P05710
C	218	HIS	-	expression tag	UNP P05710

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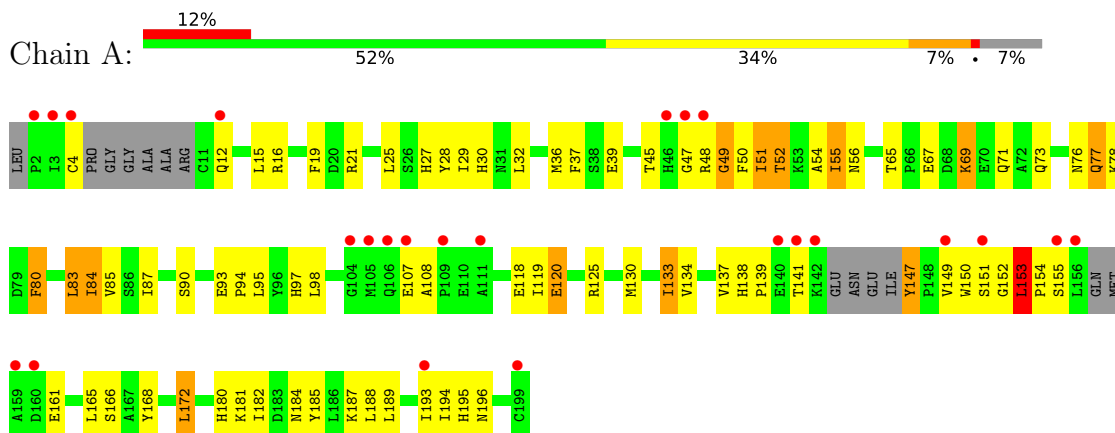
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Chain	Residue	Modelled	Actual	Comment	Reference
C	219	HIS	-	expression tag	UNP P05710
C	220	HIS	-	expression tag	UNP P05710

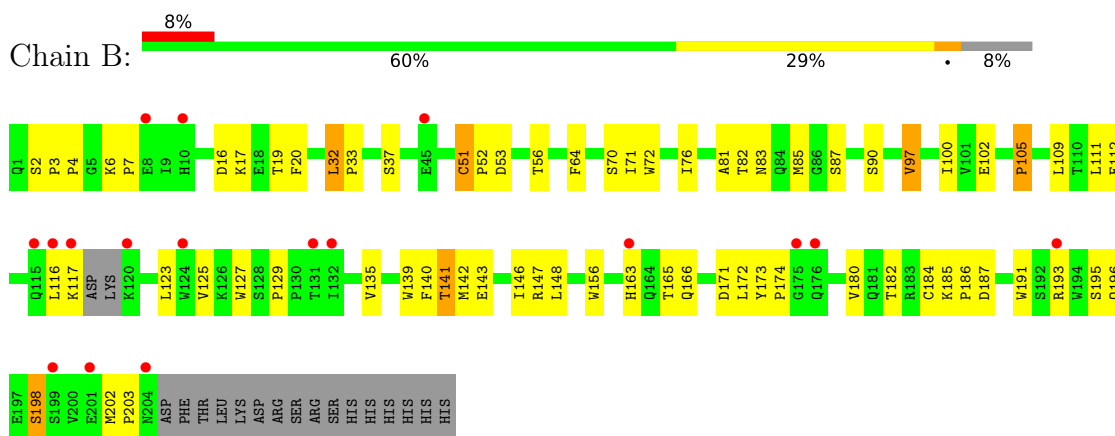
3 Residue-property plots [i](#)

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 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.

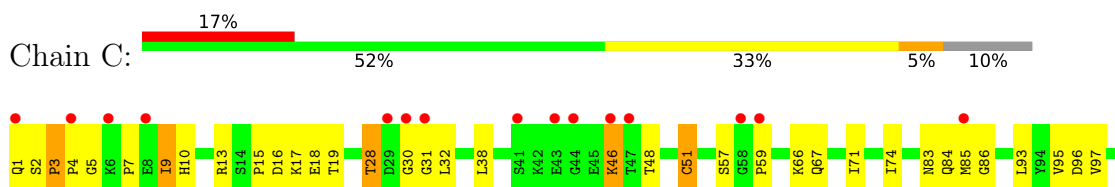
• Molecule 1: Prolactin

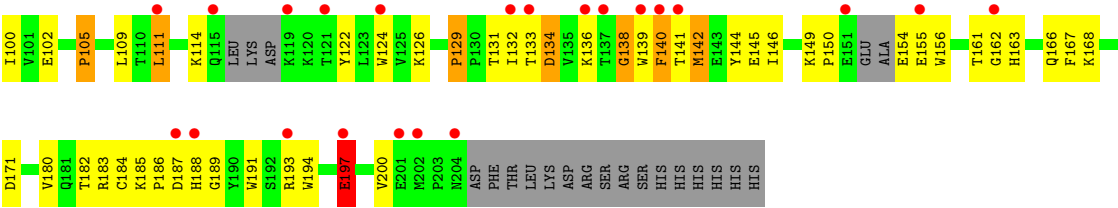


• Molecule 2: Prolactin receptor



• Molecule 2: Prolactin receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.17Å 92.17Å 216.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.78 – 3.35 84.78 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (84.78-3.35) 97.0 (84.78-3.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.234 , 0.292 0.239 , 0.224	Depositor DCC
R_{free} test set	683 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.66	0/1535	1.07	8/2071 (0.4%)
2	B	0.62	0/1724	1.04	12/2351 (0.5%)
2	C	0.57	0/1701	0.94	7/2318 (0.3%)
All	All	0.62	0/4960	1.02	27/6740 (0.4%)

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	C	0	1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	PRO	CA-C-N	9.80	129.87	119.78
2	B	105	PRO	C-N-CA	9.80	129.87	119.78
1	A	147	TYR	CA-C-N	9.51	130.10	119.83
1	A	147	TYR	C-N-CA	9.51	130.10	119.83
1	A	52	THR	N-CA-C	-7.76	101.67	112.45
1	A	108	ALA	CA-C-N	6.88	127.33	120.52
1	A	108	ALA	C-N-CA	6.88	127.33	120.52
2	B	129	PRO	CA-C-N	6.63	126.60	119.78
2	B	129	PRO	C-N-CA	6.63	126.60	119.78
2	C	129	PRO	CA-C-N	6.29	126.26	120.03
2	C	129	PRO	C-N-CA	6.29	126.26	120.03
1	A	84	ILE	CB-CA-C	-6.28	103.55	112.22
2	B	32	LEU	CA-C-N	6.10	126.04	119.76
2	B	32	LEU	C-N-CA	6.10	126.04	119.76
2	C	74	ILE	CB-CA-C	-6.10	103.58	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	GLU	CA-C-N	5.97	126.47	120.14
2	B	102	GLU	C-N-CA	5.97	126.47	120.14
1	A	153	LEU	CA-C-N	5.91	125.82	119.85
1	A	153	LEU	C-N-CA	5.91	125.82	119.85
2	C	51	CYS	CA-C-N	5.87	125.42	119.19
2	C	51	CYS	C-N-CA	5.87	125.42	119.19
2	B	6	LYS	CA-C-N	5.48	125.38	119.85
2	B	6	LYS	C-N-CA	5.48	125.38	119.85
2	C	105	PRO	O-C-N	5.15	123.68	121.31
2	B	51	CYS	CA-C-N	5.11	125.94	120.47
2	B	51	CYS	C-N-CA	5.11	125.94	120.47
2	C	95	VAL	N-CA-C	5.05	115.99	108.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	138	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	1507	0	1485	76	0
2	B	1666	0	1581	54	0
2	C	1644	0	1558	64	0
All	All	4817	0	4624	184	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 19.

All (184) 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:B:146:ILE:HG22	2:B:182:THR:HG22	1.24	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:THR:HG22	2:B:87:SER:HB3	1.26	1.10
1:A:15:LEU:HD11	1:A:133:ILE:CD1	1.90	1.02
1:A:15:LEU:HD11	1:A:133:ILE:HD13	1.40	1.00
2:C:154:GLU:HG2	2:C:155:GLU:H	1.34	0.93
2:B:142:MET:HG2	2:B:185:LYS:O	1.68	0.91
2:B:82:THR:HG22	2:B:87:SER:CB	1.99	0.91
1:A:15:LEU:CD1	1:A:133:ILE:HD13	2.05	0.87
2:B:111:LEU:HD21	2:B:180:VAL:HG11	1.63	0.79
1:A:184:ASN:HD21	2:B:17:LYS:NZ	1.83	0.76
2:C:5:GLY:C	2:C:7:PRO:HD3	2.11	0.76
1:A:52:THR:O	1:A:55:ILE:HD11	1.86	0.75
1:A:87:ILE:O	1:A:90:SER:HB3	1.87	0.73
1:A:65:THR:HG21	1:A:181:LYS:NZ	2.04	0.73
1:A:28:TYR:CZ	1:A:32:LEU:HD11	2.25	0.71
2:B:172:LEU:HD13	2:B:202:MET:HE1	1.74	0.70
2:C:124:TRP:CZ3	2:C:168:LYS:HE2	2.26	0.70
1:A:51:ILE:HA	1:A:54:ALA:HB3	1.74	0.70
2:B:146:ILE:HD12	2:B:148:LEU:HD11	1.73	0.69
2:C:5:GLY:O	2:C:7:PRO:HD3	1.92	0.69
1:A:184:ASN:HD21	2:B:17:LYS:HZ1	1.42	0.68
2:C:146:ILE:HG22	2:C:182:THR:HG22	1.76	0.68
2:C:2:SER:OG	2:C:3:PRO:CD	2.42	0.67
1:A:47:GLY:O	1:A:49:GLY:N	2.27	0.66
1:A:37:PHE:HD1	1:A:172:LEU:HB3	1.61	0.66
1:A:16:ARG:HA	1:A:194:ILE:HD13	1.79	0.64
1:A:50:PHE:O	1:A:52:THR:N	2.30	0.64
1:A:27:HIS:HD2	1:A:187:LYS:NZ	1.97	0.63
1:A:193:ILE:HG13	1:A:194:ILE:HG13	1.80	0.63
2:C:2:SER:O	2:C:4:PRO:HD3	1.97	0.63
2:C:154:GLU:HG2	2:C:155:GLU:N	2.08	0.63
2:B:2:SER:HB2	2:B:3:PRO:HD2	1.81	0.63
2:B:172:LEU:HD13	2:B:202:MET:CE	2.28	0.62
1:A:36:MET:HE3	1:A:172:LEU:HD11	1.79	0.62
1:A:187:LYS:HD3	2:B:141:THR:HG21	1.81	0.62
1:A:95:LEU:HB3	1:A:120:GLU:HG2	1.80	0.62
1:A:45:THR:HG23	1:A:50:PHE:CD2	2.34	0.62
2:C:134:ASP:O	2:C:138:GLY:HA3	2.00	0.62
2:C:46:LYS:HE3	2:C:46:LYS:HA	1.80	0.62
2:C:187:ASP:C	2:C:189:GLY:H	2.07	0.62
2:C:100:ILE:HD12	2:C:100:ILE:O	1.99	0.62
1:A:21:ARG:NH1	2:C:71:ILE:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	1:A:87:ILE:HG12	2.01	0.61
2:B:135:VAL:HG12	2:B:140:PHE:O	2.00	0.61
2:C:15:PRO:HD2	2:C:19:THR:O	2.00	0.61
1:A:36:MET:HE3	1:A:172:LEU:CD1	2.31	0.61
1:A:65:THR:HG21	1:A:181:LYS:CE	2.31	0.60
2:B:53:ASP:OD2	2:B:56:THR:OG1	2.19	0.60
1:A:50:PHE:C	1:A:52:THR:H	2.11	0.59
1:A:30:HIS:HD2	1:A:180:HIS:N	2.01	0.59
1:A:55:ILE:HD13	1:A:55:ILE:H	1.68	0.59
2:C:142:MET:HE1	2:C:186:PRO:HG3	1.84	0.59
2:C:183:ARG:HG3	2:C:194:TRP:CE3	2.38	0.58
1:A:50:PHE:C	1:A:52:THR:N	2.63	0.57
2:C:84:GLN:O	2:C:85:MET:HG2	2.05	0.57
2:C:3:PRO:HB3	2:C:83:ASN:ND2	2.20	0.57
2:C:142:MET:HG2	2:C:144:TYR:CZ	2.40	0.57
2:B:97:VAL:HA	2:B:100:ILE:HG12	1.87	0.56
2:C:139:TRP:HA	2:C:140:PHE:HB2	1.86	0.56
1:A:67:GLU:HB3	2:B:70:SER:HB2	1.85	0.56
2:C:142:MET:HG2	2:C:144:TYR:OH	2.05	0.56
2:B:146:ILE:HG22	2:B:182:THR:CG2	2.16	0.56
1:A:150:TRP:CZ2	1:A:152:GLY:HA3	2.41	0.56
1:A:125:ARG:HH12	2:C:18:GLU:HG2	1.71	0.55
2:B:116:LEU:O	2:B:117:LYS:C	2.49	0.55
2:C:162:GLY:O	2:C:163:HIS:HB2	2.07	0.55
2:C:145:GLU:OE2	2:C:183:ARG:NH2	2.36	0.55
2:C:200:VAL:HG13	2:C:200:VAL:O	2.07	0.54
2:B:142:MET:SD	2:B:184:CYS:HB2	2.48	0.54
2:C:146:ILE:O	2:C:146:ILE:HG13	2.07	0.53
1:A:19:PHE:CE1	1:A:193:ILE:HD11	2.42	0.53
2:B:71:ILE:HG22	2:B:72:TRP:N	2.24	0.53
2:C:3:PRO:CG	2:C:86:GLY:HA3	2.38	0.53
1:A:77:GLN:HE21	1:A:78:LYS:H	1.57	0.53
2:B:109:LEU:HD23	2:B:198:SER:HB2	1.90	0.52
2:B:112:GLU:O	2:B:123:LEU:HD12	2.09	0.52
2:B:135:VAL:HA	2:B:140:PHE:O	2.09	0.52
1:A:94:PRO:HD3	1:A:151:SER:HB3	1.91	0.52
2:B:20:PHE:CZ	2:B:64:PHE:CD1	2.97	0.52
2:C:105:PRO:HG3	2:C:193:ARG:HG3	1.92	0.52
1:A:119:ILE:O	1:A:120:GLU:C	2.51	0.51
1:A:153:LEU:HD11	1:A:168:TYR:CZ	2.45	0.51
2:C:28:THR:C	2:C:30:GLY:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:LEU:HG	2:B:180:VAL:HG23	1.93	0.51
2:B:116:LEU:HD12	2:B:117:LYS:N	2.25	0.51
2:C:3:PRO:O	2:C:5:GLY:N	2.41	0.50
2:B:147:ARG:HD2	2:B:156:TRP:CD2	2.45	0.50
2:B:143:GLU:HG2	2:B:163:HIS:CE1	2.46	0.50
2:C:3:PRO:HG2	2:C:86:GLY:C	2.37	0.50
2:B:16:ASP:O	2:B:17:LYS:HB3	2.12	0.50
1:A:4:CYS:HB2	1:A:12:GLN:HB2	1.94	0.50
2:C:124:TRP:HZ3	2:C:168:LYS:HE2	1.76	0.49
2:B:7:PRO:O	2:B:90:SER:HB2	2.12	0.49
2:C:109:LEU:HD21	2:C:180:VAL:HG13	1.94	0.49
1:A:30:HIS:NE2	1:A:180:HIS:HB2	2.27	0.49
2:B:186:PRO:O	2:B:187:ASP:C	2.55	0.49
2:C:131:THR:HG23	2:C:136:LYS:HE2	1.94	0.49
1:A:67:GLU:H	1:A:71:GLN:NE2	2.10	0.49
2:C:111:LEU:HD21	2:C:180:VAL:HG12	1.94	0.49
1:A:55:ILE:O	1:A:56:ASN:HB2	2.12	0.49
1:A:27:HIS:HD2	1:A:187:LYS:HZ3	1.61	0.48
1:A:45:THR:HG23	1:A:50:PHE:HD2	1.78	0.48
2:C:2:SER:OG	2:C:3:PRO:HD2	2.12	0.48
1:A:93:GLU:N	1:A:94:PRO:HD2	2.28	0.48
2:B:32:LEU:HB3	2:B:33:PRO:HD2	1.94	0.48
1:A:67:GLU:HB2	1:A:71:GLN:HE22	1.79	0.48
2:C:144:TYR:CD1	2:C:184:CYS:HB3	2.47	0.48
1:A:137:VAL:HG13	1:A:137:VAL:O	2.14	0.47
2:C:67:GLN:O	2:C:67:GLN:HG2	2.13	0.47
1:A:93:GLU:O	1:A:97:HIS:HD2	1.97	0.47
1:A:161:GLU:O	1:A:165:LEU:HD23	2.14	0.47
2:B:127:TRP:O	2:B:165:THR:HB	2.14	0.47
1:A:15:LEU:CD1	1:A:133:ILE:CD1	2.74	0.47
2:C:149:LYS:HG2	2:C:156:TRP:CZ3	2.50	0.47
2:C:197:GLU:H	2:C:197:GLU:CD	2.23	0.47
2:B:185:LYS:HG2	2:B:186:PRO:O	2.15	0.47
2:C:131:THR:CG2	2:C:136:LYS:HE2	2.44	0.47
1:A:25:LEU:O	1:A:29:ILE:HG13	2.15	0.46
2:C:2:SER:C	2:C:4:PRO:HD3	2.40	0.46
1:A:27:HIS:HD2	1:A:187:LYS:HZ1	1.64	0.46
2:B:185:LYS:HB2	2:B:191:TRP:CE3	2.50	0.46
2:B:2:SER:HA	2:B:85:MET:HG2	1.98	0.46
1:A:107:GLU:HG2	1:A:107:GLU:O	2.16	0.46
1:A:153:LEU:HD22	1:A:154:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:HD12	1:A:133:ILE:O	2.16	0.46
2:B:140:PHE:CE1	2:B:142:MET:HE2	2.51	0.46
2:C:16:ASP:O	2:C:17:LYS:HB2	2.16	0.45
2:C:138:GLY:C	2:C:139:TRP:CD1	2.94	0.45
1:A:85:VAL:HG21	1:A:134:VAL:HG21	1.99	0.45
1:A:172:LEU:HD13	1:A:172:LEU:HA	1.77	0.45
2:B:4:PRO:HD3	2:B:83:ASN:CG	2.41	0.45
2:C:9:ILE:HG21	2:C:93:LEU:HB2	1.98	0.45
1:A:37:PHE:CD1	1:A:172:LEU:HB3	2.48	0.45
1:A:65:THR:HG21	1:A:181:LYS:HZ3	1.78	0.45
1:A:69:LYS:HG3	2:B:139:TRP:CG	2.52	0.45
1:A:195:HIS:O	1:A:196:ASN:C	2.59	0.45
2:C:2:SER:OG	2:C:3:PRO:HD3	2.15	0.44
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.80	0.44
2:C:132:ILE:O	2:C:134:ASP:N	2.47	0.44
1:A:84:ILE:HD11	1:A:185:TYR:CB	2.48	0.44
2:C:126:LYS:HG3	2:C:166:GLN:HB3	1.99	0.44
2:B:171:ASP:HB2	2:C:168:LYS:H	1.83	0.44
2:C:15:PRO:HG2	2:C:16:ASP:OD1	2.17	0.44
1:A:147:TYR:CD1	1:A:147:TYR:C	2.96	0.43
2:C:129:PRO:HB3	2:C:144:TYR:OH	2.18	0.43
2:B:187:ASP:N	2:B:187:ASP:OD1	2.51	0.43
2:B:146:ILE:CD1	2:B:148:LEU:HD11	2.45	0.43
1:A:84:ILE:HG21	1:A:130:MET:HE2	2.00	0.43
1:A:87:ILE:HB	1:A:182:ILE:HD11	2.01	0.43
2:C:185:LYS:HA	2:C:186:PRO:HD3	1.77	0.43
1:A:147:TYR:CE1	1:A:149:VAL:HG22	2.54	0.43
2:C:3:PRO:CD	2:C:86:GLY:HA3	2.49	0.43
1:A:51:ILE:HA	1:A:54:ALA:CB	2.47	0.43
2:C:96:ASP:O	2:C:97:VAL:C	2.61	0.43
2:B:51:CYS:HA	2:B:52:PRO:HD3	1.65	0.43
2:B:19:THR:HB	2:B:64:PHE:O	2.18	0.42
1:A:138:HIS:HA	1:A:139:PRO:HD3	1.71	0.42
2:B:4:PRO:HD3	2:B:83:ASN:OD1	2.19	0.42
2:C:32:LEU:HD13	2:C:84:GLN:HG3	2.01	0.42
1:A:77:GLN:HE21	1:A:78:LYS:N	2.17	0.42
2:C:185:LYS:HD3	2:C:191:TRP:CE2	2.54	0.42
1:A:188:LEU:HD23	1:A:189:LEU:HD22	2.02	0.42
1:A:95:LEU:HA	1:A:95:LEU:HD23	1.77	0.42
2:B:105:PRO:HG3	2:B:193:ARG:O	2.19	0.42
2:B:195:SER:O	2:B:196:GLN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:MET:O	2:C:163:HIS:HA	2.20	0.42
1:A:187:LYS:CD	2:B:141:THR:HG21	2.48	0.41
2:C:13:ARG:HD2	2:C:102:GLU:HB2	2.02	0.41
2:B:71:ILE:CG2	2:B:72:TRP:N	2.84	0.41
2:C:1:GLN:HG3	2:C:2:SER:O	2.20	0.41
2:C:9:ILE:O	2:C:9:ILE:HG23	2.19	0.41
1:A:50:PHE:CE1	1:A:166:SER:HA	2.56	0.41
2:B:202:MET:HG3	2:B:203:PRO:HD2	2.02	0.41
2:B:173:TYR:CD1	2:B:174:PRO:HD2	2.55	0.41
2:C:114:LYS:HG2	2:C:122:TYR:OH	2.20	0.41
1:A:76:ASN:O	1:A:80:PHE:HB2	2.21	0.41
2:B:71:ILE:HD12	2:B:71:ILE:N	2.35	0.41
2:C:138:GLY:HA2	2:C:139:TRP:CD1	2.55	0.41
1:A:16:ARG:HA	1:A:194:ILE:CD1	2.50	0.41
1:A:30:HIS:CD2	1:A:180:HIS:CA	3.03	0.41
1:A:84:ILE:HD11	1:A:185:TYR:HB3	2.03	0.40
2:B:81:ALA:O	2:B:87:SER:HA	2.21	0.40
2:B:171:ASP:HB3	2:C:167:PHE:CD1	2.56	0.40
2:C:38:LEU:C	2:C:38:LEU:HD23	2.46	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	178/199 (89%)	154 (86%)	19 (11%)	5 (3%)	4	19
2	B	198/220 (90%)	182 (92%)	16 (8%)	0	100	100
2	C	193/220 (88%)	151 (78%)	30 (16%)	12 (6%)	1	7
All	All	569/639 (89%)	487 (86%)	65 (11%)	17 (3%)	3	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	155	SER
2	C	10	HIS
2	C	140	PHE
1	A	141	THR
2	C	3	PRO
2	C	28	THR
2	C	59	PRO
2	C	133	THR
2	C	141	THR
2	C	150	PRO
2	C	197	GLU
1	A	48	ARG
2	C	31	GLY
2	C	188	HIS
2	C	171	ASP
1	A	49	GLY

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	171/181 (94%)	158 (92%)	13 (8%)	12	38
2	B	189/207 (91%)	182 (96%)	7 (4%)	30	55
2	C	187/207 (90%)	176 (94%)	11 (6%)	18	44
All	All	547/595 (92%)	516 (94%)	31 (6%)	18	46

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	55	ILE
1	A	69	LYS
1	A	73	GLN
1	A	77	GLN
1	A	80	PHE

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Mol	Chain	Res	Type
1	A	83	LEU
1	A	98	LEU
1	A	118	GLU
1	A	120	GLU
1	A	133	ILE
1	A	153	LEU
1	A	172	LEU
2	B	37	SER
2	B	76	ILE
2	B	97	VAL
2	B	125	VAL
2	B	141	THR
2	B	166	GLN
2	B	198	SER
2	C	9	ILE
2	C	46	LYS
2	C	48	THR
2	C	51	CYS
2	C	57	SER
2	C	66	LYS
2	C	111	LEU
2	C	134	ASP
2	C	142	MET
2	C	161	THR
2	C	197	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	30	HIS
1	A	46	HIS
1	A	71	GLN
1	A	74	GLN
1	A	77	GLN
1	A	97	HIS
1	A	184	ASN
1	A	195	HIS
1	A	197	ASN
2	B	1	GLN
2	B	108	ASN
2	B	159	HIS

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Mol	Chain	Res	Type
2	B	163	HIS
2	B	166	GLN
2	B	188	HIS
2	C	67	GLN
2	C	84	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/199 (93%)	0.66	24 (12%) 7 8	17, 49, 117, 173	0
2	B	202/220 (91%)	0.37	17 (8%) 17 14	18, 48, 96, 128	0
2	C	199/220 (90%)	1.00	37 (18%) 3 4	37, 65, 125, 188	0
All	All	587/639 (91%)	0.67	78 (13%) 7 7	17, 55, 120, 188	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	4	PRO	4.9
1	A	156	LEU	4.9
2	C	6	LYS	4.7
1	A	104	GLY	4.6
1	A	199	CYS	4.5
2	C	151	GLU	4.2
2	C	137	THR	4.1
2	B	116	LEU	4.0
1	A	155	SER	4.0
1	A	159	ALA	4.0
1	A	105	MET	3.8
2	B	120	LYS	3.8
2	C	119	LYS	3.7
2	C	140	PHE	3.7
1	A	107	GLU	3.6
1	A	12	GLN	3.6
1	A	48	ARG	3.6
1	A	141	THR	3.6
1	A	2	PRO	3.5
2	C	115	GLN	3.5
2	C	141	THR	3.5
2	C	204	ASN	3.4
1	A	111	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	151	SER	3.4
2	C	8	GLU	3.3
2	C	58	GLY	3.3
1	A	140	GLU	3.2
2	C	46	LYS	3.1
2	C	187	ASP	3.1
2	C	31	GLY	3.1
1	A	106	GLN	3.0
2	B	117	LYS	3.0
2	C	1	GLN	3.0
2	B	10	HIS	2.9
2	C	136	LYS	2.9
1	A	4	CYS	2.8
1	A	3	ILE	2.8
1	A	160	ASP	2.7
1	A	46	HIS	2.7
2	B	163	HIS	2.7
2	B	115	GLN	2.7
1	A	47	GLY	2.7
2	B	176	GLN	2.6
2	C	59	PRO	2.6
2	C	188	HIS	2.6
2	C	155	GLU	2.5
2	B	201	GLU	2.5
2	C	201	GLU	2.5
2	C	133	THR	2.5
2	C	29	ASP	2.5
2	B	8	GLU	2.5
2	B	204	ASN	2.5
2	B	131	THR	2.5
2	C	85	MET	2.4
2	C	202	MET	2.4
2	C	121	THR	2.4
2	B	175	GLY	2.4
2	C	43	GLU	2.4
2	C	41	SER	2.3
2	C	162	GLY	2.3
2	B	45	GLU	2.3
1	A	109	PRO	2.3
2	C	139	TRP	2.2
2	B	132	ILE	2.2
2	C	44	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	124	TRP	2.2
1	A	142	LYS	2.2
2	B	199	SER	2.2
2	C	111	LEU	2.2
2	C	197	GLU	2.2
2	C	30	GLY	2.2
1	A	193	ILE	2.1
2	C	132	ILE	2.1
2	C	193	ARG	2.1
2	B	124	TRP	2.1
2	B	193	ARG	2.1
2	C	47	THR	2.1
1	A	149	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.