Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:49 PM GMT

PDB ID	:	1HGU
Title	:	HUMAN GROWTH HORMONE
Authors	:	Chantalat, L.; Jones, N.; Korber, F.; Navaza, J.; Pavlovsky, A.G.
Deposited on	:	1995-05-11
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

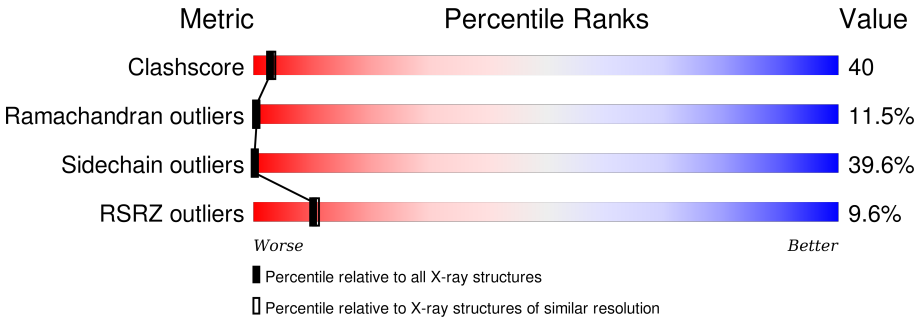
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 >=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 <=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	191	9% 21% 31% 34% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1575 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	187	Total	C	N	O	S	50	0	1
			1494	947	256	284	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLN	ASP	CONFLICT	UNP P01241
A	29	GLU	GLN	CONFLICT	UNP P01241
A	47	ALA	ASN	CONFLICT	UNP P01241
A	50	ALA	THR	CONFLICT	UNP P01241
A	66	GLN	GLU	CONFLICT	UNP P01241
A	67	ALA	THR	CONFLICT	UNP P01241
A	74	GLN	GLU	CONFLICT	UNP P01241
A	91	GLY	GLN	CONFLICT	UNP P01241
A	109	ASP	ASN	CONFLICT	UNP P01241
A	138	ALA	ILE	CONFLICT	UNP P01241
A	144	ALA	SER	CONFLICT	UNP P01241
A	148	ALA	THR	CONFLICT	UNP P01241

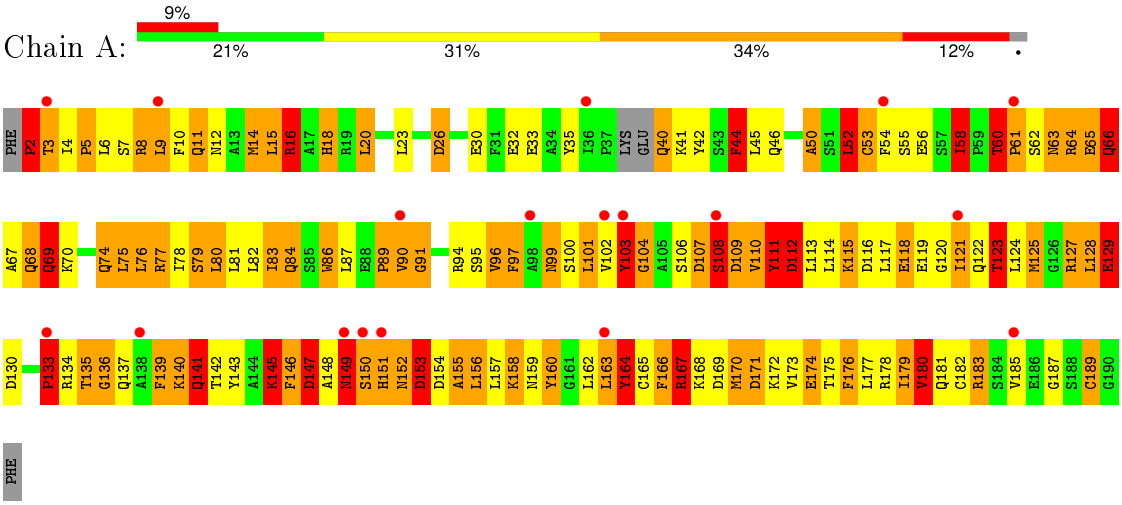
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		

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.

- Molecule 1: HUMAN GROWTH HORMONE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	57.02Å 57.02Å 130.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 42.88 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 66.0 (42.88-2.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.48Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.212 , (Not available) 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 2435.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 5359 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	1575	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.93	22/1523 (1.4%)	2.69	120/2054 (5.8%)

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
1	A	0	8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	HIS	C-N	28.63	1.99	1.34
1	A	61	PRO	C-N	26.63	1.95	1.34
1	A	180	VAL	C-N	19.81	1.79	1.34
1	A	103	TYR	CB-CG	19.70	1.81	1.51
1	A	136	GLY	C-N	-16.93	0.95	1.34
1	A	153	ASP	C-N	16.66	1.72	1.34
1	A	110	VAL	C-N	-12.47	1.05	1.34
1	A	100	SER	C-N	10.56	1.58	1.34
1	A	103	TYR	CA-CB	9.87	1.75	1.53
1	A	103	TYR	CG-CD2	9.33	1.51	1.39
1	A	103	TYR	CD2-CE2	9.16	1.53	1.39
1	A	103	TYR	C-N	-8.60	1.17	1.33
1	A	103	TYR	CG-CD1	8.24	1.49	1.39
1	A	103	TYR	CD1-CE1	7.81	1.51	1.39
1	A	183	ARG	C-N	6.53	1.49	1.34
1	A	141	GLN	C-N	5.84	1.47	1.34
1	A	180	VAL	CA-CB	5.74	1.66	1.54
1	A	3	THR	C-N	5.57	1.46	1.34
1	A	104	GLY	N-CA	-5.28	1.38	1.46
1	A	66	GLN	C-N	-5.26	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	TYR	CE2-CZ	5.26	1.45	1.38
1	A	151	HIS	CA-CB	-5.04	1.42	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ASP	O-C-N	-28.53	77.05	122.70
1	A	151	HIS	O-C-N	17.15	150.14	122.70
1	A	103	TYR	CB-CG-CD1	16.63	130.98	121.00
1	A	61	PRO	C-N-CA	-16.41	80.67	121.70
1	A	150	SER	CB-CA-C	14.60	137.84	110.10
1	A	66	GLN	O-C-N	-14.53	99.45	122.70
1	A	16	ARG	NE-CZ-NH2	-14.39	113.10	120.30
1	A	151	HIS	CA-C-N	-14.29	85.77	117.20
1	A	16	ARG	NE-CZ-NH1	14.07	127.34	120.30
1	A	149	ASN	CB-CA-C	-13.52	83.37	110.40
1	A	69	GLN	O-C-N	13.46	144.24	122.70
1	A	103	TYR	CD1-CG-CD2	-12.48	104.17	117.90
1	A	180	VAL	C-N-CA	-12.15	91.33	121.70
1	A	8	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	149	ASN	O-C-N	-10.74	105.52	122.70
1	A	69	GLN	CA-C-N	-10.45	94.21	117.20
1	A	3	THR	C-N-CA	-9.90	96.94	121.70
1	A	64	ARG	O-C-N	9.67	138.17	122.70
1	A	103	TYR	CG-CD1-CE1	9.52	128.91	121.30
1	A	167	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	136	GLY	O-C-N	-9.29	107.84	122.70
1	A	103	TYR	CB-CA-C	-9.27	91.87	110.40
1	A	18	HIS	CA-CB-CG	-9.16	98.02	113.60
1	A	134	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	58	ILE	N-CA-C	-9.10	86.44	111.00
1	A	8	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	86	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	A	189	CYS	N-CA-C	-8.61	87.76	111.00
1	A	3	THR	O-C-N	8.54	136.36	122.70
1	A	45	LEU	CA-CB-CG	8.27	134.31	115.30
1	A	103	TYR	N-CA-CB	-8.25	95.76	110.60
1	A	183	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	76	LEU	CA-C-N	8.09	134.99	117.20
1	A	143	TYR	C-N-CA	7.94	141.56	121.70
1	A	64	ARG	CA-C-N	-7.90	99.82	117.20
1	A	86	TRP	CE2-CD2-CG	-7.83	101.03	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	TYR	O-C-N	7.81	136.47	123.20
1	A	166	PHE	CB-CG-CD1	7.64	126.15	120.80
1	A	136	GLY	CA-C-N	7.60	133.93	117.20
1	A	15	LEU	CA-CB-CG	7.58	132.73	115.30
1	A	166	PHE	CB-CG-CD2	-7.54	115.52	120.80
1	A	3	THR	CA-C-N	-7.49	100.71	117.20
1	A	60	THR	CA-CB-CG2	7.37	122.71	112.40
1	A	103	TYR	CG-CD2-CE2	7.36	127.19	121.30
1	A	153	ASP	CA-C-N	7.26	133.18	117.20
1	A	66	GLN	CA-C-N	7.26	133.17	117.20
1	A	167	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	69	GLN	C-N-CA	7.00	139.21	121.70
1	A	149	ASN	CA-C-N	6.98	132.56	117.20
1	A	58	ILE	CB-CA-C	-6.92	97.75	111.60
1	A	64	ARG	CB-CA-C	-6.89	96.61	110.40
1	A	129	GLU	N-CA-C	6.87	129.56	111.00
1	A	104	GLY	C-N-CA	-6.81	104.67	121.70
1	A	63	ASN	O-C-N	-6.78	111.85	122.70
1	A	16	ARG	CG-CD-NE	6.76	126.01	111.80
1	A	151	HIS	C-N-CA	6.67	138.36	121.70
1	A	108	SER	O-C-N	-6.63	112.09	122.70
1	A	109	ASP	CB-CA-C	-6.62	97.17	110.40
1	A	2	PRO	CA-C-N	6.61	131.73	117.20
1	A	167	ARG	CA-CB-CG	6.60	127.93	113.40
1	A	136	GLY	C-N-CA	6.57	138.12	121.70
1	A	104	GLY	N-CA-C	-6.54	96.75	113.10
1	A	103	TYR	CA-C-N	-6.46	103.28	116.20
1	A	50	ALA	N-CA-C	6.44	128.38	111.00
1	A	103	TYR	CA-CB-CG	6.43	125.62	113.40
1	A	23	LEU	CB-CA-C	-6.42	98.00	110.20
1	A	147	ASP	O-C-N	-6.40	112.47	122.70
1	A	103	TYR	CB-CG-CD2	6.38	124.83	121.00
1	A	45	LEU	CB-CA-C	-6.35	98.13	110.20
1	A	53	CYS	O-C-N	-6.33	112.58	122.70
1	A	5	PRO	O-C-N	6.31	132.80	122.70
1	A	176	PHE	CB-CG-CD2	-6.26	116.42	120.80
1	A	127	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	64	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	A	104	GLY	O-C-N	-6.14	112.87	122.70
1	A	149	ASN	N-CA-C	6.10	127.47	111.00
1	A	69	GLN	N-CA-CB	-6.07	99.67	110.60
1	A	164	TYR	CB-CG-CD2	-6.06	117.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ARG	CB-CG-CD	6.06	127.36	111.60
1	A	153	ASP	CB-CA-C	-6.06	98.28	110.40
1	A	111	TYR	CA-CB-CG	6.02	124.83	113.40
1	A	76	LEU	CA-C-O	-6.01	107.47	120.10
1	A	179	ILE	CG1-CB-CG2	-5.96	98.28	111.40
1	A	66	GLN	C-N-CA	5.93	136.53	121.70
1	A	86	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	53	CYS	CA-C-N	5.92	130.22	117.20
1	A	107	ASP	O-C-N	-5.91	113.24	122.70
1	A	60	THR	CA-CB-OG1	-5.82	96.77	109.00
1	A	112	ASP	N-CA-C	5.78	126.62	111.00
1	A	75	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	A	166	PHE	CA-CB-CG	5.69	127.56	113.90
1	A	44	PHE	CB-CG-CD1	5.65	124.76	120.80
1	A	16	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	86	TRP	CB-CG-CD1	-5.64	119.67	127.00
1	A	115	LYS	CA-C-N	5.59	129.51	117.20
1	A	134	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	86	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	A	160	TYR	CA-CB-CG	5.46	123.77	113.40
1	A	158	LYS	CA-CB-CG	5.42	125.32	113.40
1	A	103	TYR	CE1-CZ-CE2	-5.37	111.21	119.80
1	A	146	PHE	O-C-N	5.34	131.24	122.70
1	A	77	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	44	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	A	171	ASP	CA-CB-CG	5.25	124.95	113.40
1	A	16	ARG	CB-CG-CD	-5.24	97.97	111.60
1	A	53	CYS	CA-CB-SG	5.23	123.41	114.00
1	A	125	MET	CB-CG-SD	-5.21	96.76	112.40
1	A	185	VAL	CB-CA-C	-5.21	101.50	111.40
1	A	136	GLY	N-CA-C	5.18	126.06	113.10
1	A	40	GLN	CA-CB-CG	-5.17	102.02	113.40
1	A	100	SER	CA-C-N	-5.17	105.83	117.20
1	A	153	ASP	C-N-CA	5.16	134.61	121.70
1	A	100	SER	O-C-N	5.13	130.91	122.70
1	A	42	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	140	LYS	O-C-N	5.08	130.82	122.70
1	A	135	THR	N-CA-CB	-5.03	100.75	110.30
1	A	103	TYR	CD1-CE1-CZ	5.02	124.32	119.80
1	A	165	CYS	CA-C-N	5.02	128.25	117.20
1	A	63	ASN	N-CA-C	-5.01	97.46	111.00
1	A	100	SER	C-N-CA	-5.01	109.17	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	GLY	Mainchain
1	A	107	ASP	Peptide
1	A	108	SER	Peptide
1	A	141	GLN	Mainchain
1	A	149	ASN	Peptide
1	A	66	GLN	Mainchain
1	A	67	ALA	Peptide
1	A	68	GLN	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	1494	0	1453	113	0
2	A	81	0	0	2	2
All	All	1575	0	1453	113	2

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 40.

All (113) 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:103:TYR:CB	1:A:103:TYR:CA	1.75	1.60
1:A:103:TYR:CG	1:A:103:TYR:CB	1.81	1.59
1:A:153:ASP:C	1:A:154:ASP:N	1.72	1.40
1:A:180:VAL:C	1:A:181:GLN:N	1.79	1.34
1:A:151:HIS:C	1:A:152:ASN:N	1.99	1.13
1:A:153:ASP:O	1:A:154:ASP:N	1.89	1.05
1:A:103:TYR:C	1:A:103:TYR:CB	2.31	0.97
1:A:180:VAL:C	1:A:181:GLN:CA	2.34	0.96
1:A:103:TYR:CB	1:A:103:TYR:N	2.39	0.85
1:A:4:ILE:N	1:A:5:PRO:HD2	1.92	0.85
1:A:151:HIS:CG	1:A:151:HIS:O	2.28	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:O	1:A:70:LYS:HG3	1.79	0.82
1:A:151:HIS:CA	1:A:152:ASN:N	2.42	0.81
1:A:84:GLN:HA	1:A:87:LEU:HD12	1.64	0.78
1:A:97:PHE:CD2	1:A:148:ALA:HB3	2.19	0.77
1:A:77:ARG:NH1	1:A:137:GLN:O	2.19	0.76
1:A:2:PRO:O	1:A:4:ILE:N	2.19	0.76
1:A:26:ASP:OD1	1:A:102:VAL:HB	1.85	0.76
1:A:151:HIS:ND1	1:A:151:HIS:O	2.20	0.73
1:A:52:LEU:HD13	1:A:145:LYS:NZ	2.03	0.73
1:A:4:ILE:N	1:A:5:PRO:CD	2.53	0.71
1:A:68:GLN:O	1:A:70:LYS:CG	2.38	0.71
1:A:172:LYS:O	1:A:176:PHE:HB2	1.91	0.70
1:A:180:VAL:C	1:A:181:GLN:HA	2.10	0.70
1:A:117:LEU:O	1:A:121:ILE:HB	1.91	0.69
1:A:87:LEU:HD11	1:A:118:GLU:HG2	1.75	0.69
1:A:101:LEU:HD23	1:A:101:LEU:N	2.09	0.67
1:A:151:HIS:HA	1:A:152:ASN:N	2.10	0.67
1:A:164:TYR:HE1	1:A:167:ARG:HD3	1.60	0.65
1:A:124:LEU:O	1:A:128:LEU:HD12	1.96	0.65
1:A:77:ARG:NH1	1:A:135:THR:HG23	2.12	0.65
1:A:171:ASP:O	1:A:175:THR:HB	1.98	0.64
1:A:179:ILE:O	1:A:183:ARG:HB2	1.98	0.62
1:A:155:ALA:O	1:A:158:LYS:HB2	2.00	0.61
1:A:63:ASN:O	1:A:65:GLU:N	2.33	0.61
1:A:12:ASN:HD21	1:A:16:ARG:NH2	1.98	0.61
1:A:187:GLY:HA3	2:A:218:HOH:O	2.00	0.60
1:A:156:LEU:HA	1:A:159:ASN:HB2	1.83	0.60
1:A:9:LEU:HB3	1:A:124:LEU:HD21	1.83	0.60
1:A:4:ILE:O	1:A:5:PRO:C	2.39	0.60
1:A:118:GLU:HA	1:A:121:ILE:HG22	1.85	0.59
1:A:153:ASP:O	1:A:154:ASP:CA	2.51	0.59
1:A:2:PRO:C	1:A:4:ILE:H	2.05	0.59
1:A:87:LEU:HA	1:A:90:VAL:HG22	1.85	0.58
1:A:129:GLU:O	1:A:133:PRO:HB3	2.04	0.57
1:A:60:THR:OG1	1:A:172:LYS:HD3	2.04	0.57
1:A:52:LEU:HD13	1:A:145:LYS:HZ1	1.67	0.57
1:A:151:HIS:CD2	1:A:151:HIS:H	2.21	0.56
1:A:164:TYR:CE1	1:A:167:ARG:HD3	2.39	0.56
1:A:112:ASP:HA	1:A:115:LYS:HB2	1.86	0.56
1:A:187:GLY:CA	2:A:218:HOH:O	2.54	0.56
1:A:84:GLN:HA	1:A:87:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:O	1:A:181:GLN:HA	2.06	0.55
1:A:178:ARG:O	1:A:181:GLN:N	2.40	0.55
1:A:53:CYS:SG	1:A:168:LYS:HD3	2.47	0.54
1:A:139:PHE:O	1:A:141:GLN:HG2	2.09	0.53
1:A:83:ILE:O	1:A:87:LEU:HG	2.08	0.53
1:A:146:PHE:O	1:A:147:ASP:HB2	2.07	0.53
1:A:172:LYS:HG2	1:A:176:PHE:CE2	2.44	0.53
1:A:97:PHE:CG	1:A:148:ALA:HB3	2.44	0.52
1:A:2:PRO:C	1:A:4:ILE:N	2.60	0.52
1:A:147:ASP:OD1	1:A:148:ALA:N	2.42	0.52
1:A:178:ARG:HG2	1:A:182:CYS:SG	2.49	0.51
1:A:86:TRP:CZ2	1:A:166:PHE:HB2	2.45	0.51
1:A:32:GLU:HG3	1:A:33:GLU:N	2.25	0.51
1:A:75:LEU:HD21	1:A:183:ARG:NH1	2.25	0.50
1:A:79:SER:O	1:A:81:LEU:N	2.45	0.50
1:A:77:ARG:HD2	1:A:135:THR:OG1	2.11	0.49
1:A:32:GLU:OE1	1:A:41:LYS:HE2	2.13	0.49
1:A:7:SER:HA	1:A:10:PHE:HD2	1.77	0.49
1:A:90:VAL:HG21	1:A:114:LEU:HD13	1.95	0.49
1:A:164:TYR:O	1:A:167:ARG:HB3	2.12	0.49
1:A:111:TYR:O	1:A:113:LEU:N	2.46	0.48
1:A:6:LEU:O	1:A:9:LEU:HB2	2.14	0.48
1:A:174:GLU:O	1:A:178:ARG:N	2.47	0.48
1:A:176:PHE:HA	1:A:179:ILE:HG13	1.97	0.47
1:A:16:ARG:O	1:A:20:LEU:HB2	2.16	0.46
1:A:12:ASN:O	1:A:16:ARG:HD2	2.16	0.46
1:A:76:LEU:HD23	1:A:177:LEU:HD21	1.97	0.45
1:A:61:PRO:HG2	1:A:176:PHE:CZ	2.52	0.45
1:A:52:LEU:HD13	1:A:145:LYS:HZ2	1.78	0.45
1:A:156:LEU:O	1:A:159:ASN:HB2	2.17	0.45
1:A:75:LEU:HD21	1:A:183:ARG:HH12	1.80	0.45
1:A:66:GLN:HG2	1:A:179:ILE:CG2	2.47	0.45
1:A:30:GLU:OE2	1:A:101:LEU:HB2	2.16	0.45
1:A:170:MET:HA	1:A:173:VAL:HG23	1.99	0.45
1:A:75:LEU:O	1:A:79:SER:HB2	2.18	0.44
1:A:120:GLY:O	1:A:123:THR:HG22	2.17	0.44
1:A:76:LEU:HD23	1:A:121:ILE:HD11	2.00	0.44
1:A:149:ASN:ND2	1:A:149:ASN:N	2.67	0.43
1:A:175:THR:O	1:A:178:ARG:HB3	2.18	0.43
1:A:154:ASP:O	1:A:157:LEU:N	2.50	0.43
1:A:97:PHE:CD1	1:A:159:ASN:OD1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:O	1:A:122:GLN:HB2	2.18	0.43
1:A:35:TYR:CD1	1:A:156:LEU:HD13	2.54	0.42
1:A:69:GLN:HE21	1:A:69:GLN:HB3	1.67	0.42
1:A:80:LEU:HG	1:A:84:GLN:HG3	2.01	0.42
1:A:74:GLN:O	1:A:78:ILE:N	2.50	0.42
1:A:89:PRO:O	1:A:91:GLY:N	2.52	0.42
1:A:35:TYR:CE1	1:A:156:LEU:HD13	2.55	0.42
1:A:66:GLN:HG2	1:A:179:ILE:HG22	2.02	0.42
1:A:12:ASN:HD21	1:A:16:ARG:HH21	1.66	0.42
1:A:115:LYS:O	1:A:118:GLU:HG3	2.20	0.42
1:A:154:ASP:O	1:A:156:LEU:N	2.53	0.41
1:A:87:LEU:HA	1:A:90:VAL:CG2	2.49	0.41
1:A:97:PHE:CD2	1:A:148:ALA:CB	2.98	0.41
1:A:101:LEU:O	1:A:103:TYR:CD1	2.74	0.41
1:A:58:ILE:HD12	1:A:61:PRO:CG	2.50	0.41
1:A:95:SER:O	1:A:99:ASN:N	2.54	0.41
1:A:11:GLN:O	1:A:14:MET:N	2.54	0.41
1:A:163:LEU:HA	1:A:163:LEU:HD13	1.74	0.41
1:A:130:ASP:O	1:A:133:PRO:HD3	2.21	0.40
1:A:83:ILE:CG2	1:A:84:GLN:N	2.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:267:HOH:O	2:A:267:HOH:O[7_556]	1.70	0.50
2:A:203:HOH:O	2:A:204:HOH:O[8_665]	2.12	0.08

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	183/191 (96%)	120 (66%)	42 (23%)	21 (12%)	0 0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ALA
1	A	80	LEU
1	A	112	ASP
1	A	129	GLU
1	A	136	GLY
1	A	139	PHE
1	A	147	ASP
1	A	150	SER
1	A	52	LEU
1	A	89	PRO
1	A	90	VAL
1	A	106	SER
1	A	133	PRO
1	A	155	ALA
1	A	60	THR
1	A	123	THR
1	A	91	GLY
1	A	145	LYS
1	A	189	CYS
1	A	44	PHE
1	A	96	VAL

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	164/169 (97%)	99 (60%)	65 (40%)	0 0

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	3	THR
1	A	8	ARG
1	A	9	LEU
1	A	11	GLN
1	A	14	MET
1	A	15	LEU
1	A	16	ARG
1	A	18	HIS
1	A	20	LEU
1	A	26	ASP
1	A	40	GLN
1	A	44	PHE
1	A	46	GLN
1	A	52	LEU
1	A	54	PHE
1	A	55	SER
1	A	56	GLU
1	A	58	ILE
1	A	60	THR
1	A	62	SER
1	A	64	ARG
1	A	65	GLU
1	A	69	GLN
1	A	74	GLN
1	A	79	SER
1	A	82	LEU
1	A	83	ILE
1	A	84	GLN
1	A	94	ARG
1	A	96	VAL
1	A	97	PHE
1	A	99	ASN
1	A	101	LEU
1	A	103	TYR
1	A	108	SER
1	A	109	ASP
1	A	110	VAL
1	A	111	TYR
1	A	112	ASP
1	A	116	ASP
1	A	118	GLU
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	123	THR
1	A	125	MET
1	A	127	ARG
1	A	128	LEU
1	A	133	PRO
1	A	140	LYS
1	A	141	GLN
1	A	142	THR
1	A	145	LYS
1	A	149	ASN
1	A	152	ASN
1	A	153	ASP
1	A	156	LEU
1	A	160	TYR
1	A	162	LEU
1	A	163	LEU
1	A	164	TYR
1	A	167	ARG
1	A	169	ASP
1	A	170	MET
1	A	174	GLU
1	A	180	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	69	GLN
1	A	149	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	187/191 (97%)	0.46	18 (9%)	10	11	13, 35, 48, 56	20 (10%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	PRO	12.7
1	A	163	LEU	5.7
1	A	36	ILE	5.2
1	A	54	PHE	4.9
1	A	150	SER	4.8
1	A	185	VAL	4.3
1	A	108	SER	4.3
1	A	90	VAL	3.7
1	A	149	ASN	3.3
1	A	133	PRO	3.3
1	A	98	ALA	3.2
1	A	9	LEU	3.1
1	A	138	ALA	3.0
1	A	3	THR	2.7
1	A	121	ILE	2.2
1	A	103	TYR	2.2
1	A	151	HIS	2.2
1	A	102	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.