



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:18 am GMT

PDB ID : 1BP3
Title : THE XRAY STRUCTURE OF A GROWTH HORMONE-PROLACTIN RE-
CEPTOR COMPLEX
Authors : Somers, W.; Ultsch, M.; De Vos, A.M.; Kossiakoff, A.A.
Deposited on : 1998-08-12
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

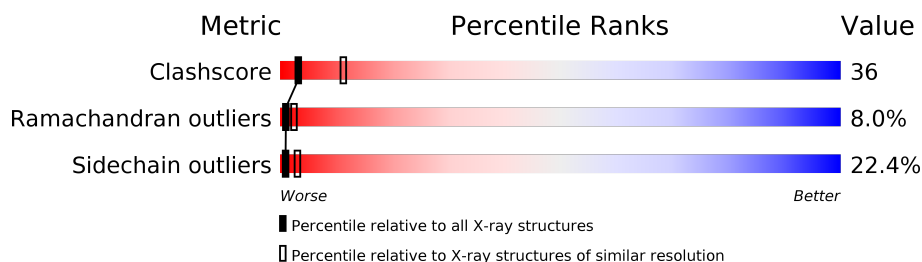
1 Overall quality at a glance

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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (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 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 $\leq 5\%$. 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	191	
2	B	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3123 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 PROTEIN (GROWTH HORMONE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1509	961	254	287	7			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called PROTEIN (PROLACTIN RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1613	1049	264	291	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

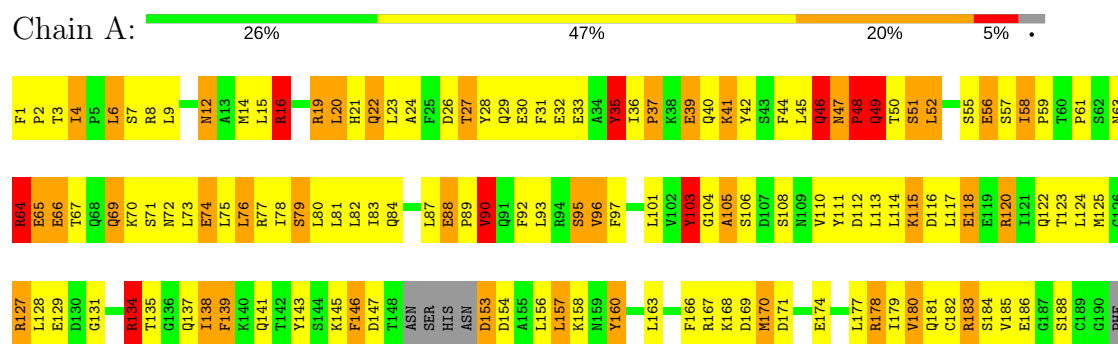
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (GROWTH HORMONE)



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	154.20Å 69.80Å 43.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.0 (10.00-2.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.11	2/1539 (0.1%)	2.17	70/2079 (3.4%)
2	B	1.16	2/1672 (0.1%)	2.26	74/2283 (3.2%)
All	All	1.14	4/3211 (0.1%)	2.22	144/4362 (3.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	338	GLY	N-CA	-7.75	1.34	1.46
1	A	131	GLY	N-CA	-5.62	1.37	1.46
2	B	258	GLY	N-CA	5.17	1.53	1.46
1	A	37	PRO	C-O	5.11	1.33	1.23

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	383	ARG	NE-CZ-NH2	-15.57	112.51	120.30
2	B	245	GLU	C-N-CA	13.80	156.19	121.70
2	B	337	THR	C-N-CA	13.70	151.07	122.30
1	A	64	ARG	NE-CZ-NH1	13.01	126.81	120.30
1	A	16	ARG	CD-NE-CZ	12.81	141.53	123.60
1	A	127	ARG	CD-NE-CZ	12.69	141.37	123.60
2	B	345	GLU	CA-CB-CG	12.08	139.99	113.40
1	A	120	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	127	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	A	178	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	A	183	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	A	33	GLU	CA-CB-CG	10.79	137.14	113.40
2	B	244	GLY	C-N-CA	10.77	148.62	121.70
2	B	348	LEU	CA-CB-CG	10.69	139.88	115.30
2	B	299	TYR	CB-CG-CD2	10.51	127.30	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	347	ARG	NE-CZ-NH1	-10.43	115.09	120.30
2	B	242	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	16	ARG	NE-CZ-NH1	9.86	125.23	120.30
2	B	383	ARG	NE-CZ-NH1	9.62	125.11	120.30
2	B	366	GLU	CA-CB-CG	9.61	134.54	113.40
2	B	318	ASP	CB-CG-OD1	9.55	126.89	118.30
1	A	64	ARG	CG-CD-NE	8.93	130.56	111.80
2	B	225	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	182	CYS	CA-CB-SG	-8.60	98.53	114.00
2	B	229	ASP	CB-CG-OD1	8.48	125.93	118.30
2	B	229	ASP	CB-CA-C	8.33	127.06	110.40
2	B	254	TYR	CB-CG-CD2	8.25	125.95	121.00
2	B	240	TYR	CB-CG-CD1	8.15	125.89	121.00
1	A	101	LEU	C-N-CA	8.15	142.07	121.70
2	B	318	ASP	CB-CA-C	8.12	126.64	110.40
2	B	334	ASP	CB-CG-OD1	-8.10	111.01	118.30
1	A	103	TYR	CB-CG-CD1	8.09	125.85	121.00
1	A	131	GLY	N-CA-C	8.07	133.28	113.10
2	B	273	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	174	GLU	CG-CD-OE2	7.98	134.25	118.30
1	A	19	ARG	CD-NE-CZ	7.90	134.66	123.60
2	B	304	ASP	CB-CG-OD1	7.87	125.39	118.30
2	B	227	GLY	C-N-CA	7.87	141.38	121.70
1	A	103	TYR	CB-CG-CD2	-7.84	116.30	121.00
1	A	139	PHE	CB-CA-C	7.71	125.82	110.40
2	B	296	ASP	CB-CG-OD1	7.70	125.23	118.30
2	B	225	ARG	NE-CZ-NH1	7.57	124.08	120.30
2	B	253	ASP	CB-CG-OD2	7.51	125.06	118.30
2	B	347	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	B	387	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	39	GLU	CA-CB-CG	7.32	129.49	113.40
1	A	127	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	120	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	127	ARG	CG-CD-NE	7.00	126.50	111.80
2	B	347	ARG	CG-CD-NE	6.94	126.37	111.80
1	A	64	ARG	NE-CZ-NH2	-6.93	116.83	120.30
2	B	337	THR	CA-C-O	6.81	134.41	120.10
2	B	236	TYR	N-CA-CB	6.81	122.85	110.60
1	A	37	PRO	N-CA-C	6.73	129.61	112.10
2	B	224	TRP	N-CA-CB	6.73	122.72	110.60
1	A	183	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	B	317	GLU	N-CA-CB	6.71	122.67	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	370	LEU	C-N-CA	6.67	138.38	121.70
1	A	56	GLU	CB-CG-CD	6.61	132.06	114.20
1	A	88	GLU	OE1-CD-OE2	6.58	131.19	123.30
2	B	208	GLU	CB-CG-CD	6.57	131.93	114.20
1	A	29	GLN	CA-CB-CG	6.56	127.84	113.40
2	B	341	THR	N-CA-CB	6.56	122.76	110.30
1	A	35	TYR	CB-CG-CD2	6.48	124.89	121.00
2	B	282	THR	N-CA-C	6.46	128.43	111.00
1	A	182	CYS	C-N-CA	6.39	137.66	121.70
1	A	26	ASP	CB-CA-C	6.30	123.01	110.40
2	B	342	LEU	CB-CA-C	6.29	122.15	110.20
1	A	39	GLU	CB-CG-CD	6.24	131.05	114.20
1	A	95	SER	CA-CB-OG	6.22	128.00	111.20
2	B	296	ASP	CA-CB-CG	6.17	126.98	113.40
2	B	253	ASP	OD1-CG-OD2	-6.14	111.63	123.30
2	B	254	TYR	N-CA-CB	6.14	121.65	110.60
1	A	58	ILE	CB-CA-C	-6.13	99.34	111.60
2	B	254	TYR	CA-CB-CG	6.09	124.97	113.40
1	A	8	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	167	ARG	CD-NE-CZ	-6.08	115.09	123.60
2	B	236	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	46	GLN	CB-CG-CD	6.00	127.21	111.60
2	B	214	SER	N-CA-CB	-6.00	101.49	110.50
1	A	26	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	57	SER	C-N-CA	5.99	136.68	121.70
1	A	46	GLN	CA-CB-CG	5.98	126.56	113.40
1	A	157	LEU	C-N-CA	5.94	136.56	121.70
1	A	154	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	153	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	112	ASP	CB-CG-OD1	-5.89	113.00	118.30
2	B	224	TRP	O-C-N	5.85	132.06	122.70
1	A	22	GLN	CG-CD-OE1	-5.83	109.93	121.60
2	B	385	LYS	O-C-N	5.83	132.18	121.10
2	B	372	LEU	C-N-CA	5.79	136.18	121.70
1	A	138	ILE	C-N-CA	-5.79	107.22	121.70
1	A	174	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	154	ASP	CB-CG-OD1	5.73	123.45	118.30
2	B	248	MET	N-CA-CB	5.70	120.85	110.60
1	A	170	MET	CB-CA-C	5.67	121.75	110.40
1	A	58	ILE	N-CA-CB	5.67	123.84	110.80
2	B	205	GLY	CA-C-N	5.67	129.67	117.20
1	A	153	ASP	CA-CB-CG	5.67	125.86	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	324	TRP	CA-CB-CG	-5.63	103.00	113.70
2	B	322	TYR	CG-CD1-CE1	5.61	125.79	121.30
2	B	268	TYR	CA-CB-CG	-5.59	102.79	113.40
2	B	338	GLY	N-CA-C	5.57	127.03	113.10
2	B	253	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	37	PRO	CA-C-N	5.54	129.39	117.20
1	A	30	GLU	CA-CB-CG	5.54	125.58	113.40
1	A	169	ASP	CB-CG-OD1	5.52	123.27	118.30
2	B	252	PRO	N-CA-C	5.48	126.36	112.10
1	A	160	TYR	CB-CG-CD2	-5.41	117.75	121.00
2	B	230	GLY	CA-C-O	5.37	130.26	120.60
2	B	258	GLY	N-CA-C	-5.37	99.69	113.10
2	B	218	GLU	O-C-N	-5.33	114.17	122.70
2	B	261	SER	O-C-N	5.33	131.22	122.70
1	A	171	ASP	CA-CB-CG	5.29	125.04	113.40
2	B	211	LYS	CA-C-O	5.29	131.20	120.10
1	A	65	GLU	OE1-CD-OE2	5.28	129.64	123.30
1	A	35	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	A	90	VAL	C-N-CA	5.27	134.87	121.70
2	B	291	ASP	CA-C-O	-5.22	109.13	120.10
1	A	69	GLN	N-CA-CB	5.22	120.00	110.60
1	A	183	ARG	CG-CD-NE	5.22	122.77	111.80
2	B	347	ARG	CD-NE-CZ	-5.22	116.30	123.60
1	A	66	GLU	CA-CB-CG	5.21	124.86	113.40
2	B	317	GLU	C-N-CA	-5.21	108.68	121.70
2	B	349	LYS	N-CA-CB	5.18	119.93	110.60
2	B	216	ASN	CA-C-N	5.18	128.60	117.20
2	B	376	GLN	CB-CG-CD	5.18	125.06	111.60
2	B	317	GLU	CG-CD-OE2	5.17	128.64	118.30
2	B	267	GLN	CB-CG-CD	5.15	125.00	111.60
1	A	171	ASP	CB-CG-OD1	5.14	122.93	118.30
2	B	205	GLY	CA-C-O	-5.12	111.38	120.60
1	A	19	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	B	282	THR	N-CA-CB	-5.09	100.62	110.30
2	B	249	HIS	CA-CB-CG	5.09	122.25	113.60
2	B	256	THR	CA-C-N	5.07	126.33	116.20
1	A	69	GLN	CA-C-O	-5.06	109.48	120.10
1	A	76	LEU	CA-CB-CG	5.04	126.90	115.30
2	B	211	LYS	CD-CE-NZ	-5.04	100.10	111.70
1	A	29	GLN	OE1-CD-NE2	-5.04	110.31	121.90
2	B	213	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	134	ARG	CA-CB-CG	5.04	124.48	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLU	CG-CD-OE1	-5.02	108.26	118.30
2	B	366	GLU	N-CA-CB	5.02	119.64	110.60
1	A	138	ILE	CA-C-N	5.01	128.22	117.20

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	1509	0	1474	107	0
2	B	1613	0	1530	121	0
3	A	1	0	0	0	0
All	All	3123	0	3004	223	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 36.

All (223) 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:378:TYR:HE1	2:B:402:ILE:HD11	1.12	1.13
1:A:46:GLN:HE22	1:A:49:GLN:HB3	1.19	1.07
2:B:270:SER:HB3	2:B:273:ARG:HG3	1.44	0.99
2:B:378:TYR:CE1	2:B:402:ILE:HD11	2.01	0.95
1:A:36:ILE:HG12	1:A:156:LEU:HD23	1.49	0.92
1:A:19:ARG:HH22	1:A:104:GLY:HA3	1.34	0.91
2:B:247:LEU:HD12	2:B:247:LEU:H	1.34	0.91
2:B:374:PRO:HB3	2:B:404:SER:HB3	1.52	0.89
1:A:88:GLU:HB2	1:A:89:PRO:HD3	1.56	0.87
1:A:64:ARG:HD2	2:B:218:GLU:OE2	1.75	0.85
1:A:35:TYR:HB3	1:A:156:LEU:HD21	1.57	0.84
2:B:278:MET:HG3	2:B:291:ASP:O	1.81	0.80
1:A:135:THR:HA	1:A:139:PHE:HE1	1.48	0.79
1:A:77:ARG:HH21	1:A:134:ARG:HH21	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:SER:HB2	1:A:113:LEU:HD11	1.64	0.77
2:B:206:LYS:HD3	2:B:228:THR:HB	1.67	0.75
2:B:238:LEU:HB3	2:B:251:CYS:HB2	1.67	0.74
1:A:16:ARG:HB2	1:A:117:LEU:HD13	1.69	0.74
1:A:96:VAL:HG11	1:A:163:LEU:HD11	1.70	0.72
2:B:203:PRO:HB2	2:B:204:PRO:HD3	1.71	0.71
2:B:327:TRP:CZ3	2:B:346:ILE:HD11	2.25	0.71
2:B:313:VAL:HG21	2:B:403:PRO:CD	2.21	0.71
1:A:31:PHE:CE1	1:A:160:TYR:HB2	2.25	0.70
1:A:84:GLN:HA	1:A:87:LEU:HD12	1.72	0.70
2:B:311:VAL:HG12	2:B:400:ILE:HD12	1.72	0.70
1:A:79:SER:O	1:A:83:ILE:HG12	1.92	0.70
1:A:36:ILE:N	1:A:37:PRO:HD3	2.06	0.70
1:A:70:LYS:HB3	1:A:74:GLU:HB3	1.74	0.69
2:B:332:LEU:HD12	2:B:333:ILE:HG12	1.75	0.68
2:B:282:THR:HG22	2:B:288:SER:HA	1.76	0.68
1:A:146:PHE:HE2	1:A:158:LYS:HE3	1.59	0.67
1:A:88:GLU:HB2	1:A:89:PRO:CD	2.24	0.66
1:A:84:GLN:HA	1:A:87:LEU:CD1	2.24	0.66
2:B:247:LEU:CD1	2:B:247:LEU:H	2.05	0.65
1:A:22:GLN:OE1	2:B:388:HIS:HE1	1.79	0.64
1:A:73:LEU:HD21	1:A:129:GLU:OE1	1.98	0.64
2:B:282:THR:HA	2:B:287:SER:O	1.97	0.63
2:B:349:LYS:HG3	2:B:353:ALA:HB3	1.80	0.63
1:A:63:ASN:OD1	1:A:66:GLU:N	2.30	0.61
2:B:250:GLU:HG3	2:B:251:CYS:N	2.15	0.61
1:A:76:LEU:HD11	1:A:128:LEU:HD12	1.83	0.61
2:B:208:GLU:O	2:B:225:ARG:N	2.34	0.60
2:B:400:ILE:HG12	2:B:401:GLN:H	1.67	0.60
2:B:275:TYR:HB2	2:B:295:VAL:HG13	1.83	0.60
2:B:304:ASP:O	2:B:330:PRO:HG3	2.01	0.60
1:A:31:PHE:HE1	1:A:160:TYR:HB2	1.66	0.60
2:B:383:ARG:HD2	2:B:394:TRP:CH2	2.37	0.59
2:B:313:VAL:HG21	2:B:403:PRO:HD3	1.83	0.59
1:A:70:LYS:O	1:A:75:LEU:HG	2.02	0.59
2:B:206:LYS:CD	2:B:228:THR:HB	2.33	0.58
2:B:311:VAL:CG1	2:B:400:ILE:HD12	2.32	0.58
1:A:66:GLU:HA	1:A:69:GLN:HB2	1.85	0.58
2:B:351:GLU:N	2:B:377:LYS:O	2.34	0.57
1:A:76:LEU:HD13	1:A:125:MET:HA	1.85	0.57
2:B:366:GLU:O	2:B:367:PHE:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:ARG:HD2	2:B:394:TRP:CZ3	2.40	0.57
2:B:350:PRO:HA	2:B:378:TYR:HA	1.85	0.57
1:A:181:GLN:O	1:A:185:VAL:HB	2.04	0.57
2:B:241:HIS:CD2	2:B:248:MET:SD	2.98	0.57
1:A:72:ASN:OD1	1:A:183:ARG:NH2	2.38	0.56
1:A:35:TYR:N	1:A:35:TYR:CD1	2.73	0.56
1:A:19:ARG:NH2	1:A:104:GLY:HA3	2.14	0.56
1:A:96:VAL:CG1	1:A:163:LEU:HD11	2.35	0.56
1:A:12:ASN:O	1:A:16:ARG:NH1	2.37	0.56
1:A:42:TYR:HD2	1:A:45:LEU:HD13	1.70	0.56
2:B:211:LYS:HG3	2:B:223:TRP:HE3	1.71	0.56
1:A:122:GLN:O	1:A:125:MET:HB3	2.06	0.55
2:B:209:ILE:HD11	2:B:279:VAL:HG23	1.87	0.55
2:B:374:PRO:HA	2:B:403:PRO:O	2.06	0.55
1:A:22:GLN:OE1	2:B:388:HIS:CE1	2.59	0.55
2:B:347:ARG:HG3	2:B:356:TRP:CE3	2.41	0.55
1:A:19:ARG:NH2	1:A:103:TYR:O	2.40	0.55
2:B:313:VAL:HG21	2:B:403:PRO:HD2	1.87	0.55
1:A:93:LEU:HA	1:A:96:VAL:HG23	1.89	0.55
2:B:240:TYR:HA	2:B:276:ILE:O	2.07	0.55
1:A:46:GLN:NE2	1:A:49:GLN:HB3	2.04	0.54
1:A:146:PHE:CG	1:A:147:ASP:N	2.75	0.54
1:A:45:LEU:HA	1:A:51:SER:HB2	1.88	0.54
2:B:209:ILE:HA	2:B:224:TRP:HA	1.89	0.54
2:B:347:ARG:HG3	2:B:356:TRP:CZ3	2.43	0.54
1:A:79:SER:O	1:A:82:LEU:HB2	2.08	0.53
1:A:84:GLN:O	1:A:87:LEU:HB2	2.08	0.53
2:B:347:ARG:CG	2:B:381:GLN:HG3	2.39	0.53
1:A:20:LEU:HD21	1:A:113:LEU:HB2	1.91	0.53
1:A:35:TYR:O	1:A:36:ILE:HB	2.07	0.53
1:A:36:ILE:CG1	1:A:156:LEU:HD23	2.30	0.53
2:B:347:ARG:HD3	2:B:394:TRP:CE2	2.44	0.52
1:A:64:ARG:HD2	2:B:218:GLU:CD	2.29	0.52
1:A:70:LYS:HD2	1:A:137:GLN:OE1	2.09	0.52
1:A:48:PRO:O	1:A:52:LEU:HD22	2.10	0.52
2:B:252:PRO:HD2	2:B:262:CYS:SG	2.50	0.51
2:B:215:PRO:O	2:B:332:LEU:HD13	2.10	0.51
2:B:225:ARG:NH1	2:B:260:ASN:HD22	2.07	0.51
2:B:376:GLN:O	2:B:402:ILE:HD12	2.11	0.51
2:B:322:TYR:HD1	2:B:323:LEU:O	1.94	0.51
1:A:76:LEU:CD1	1:A:128:LEU:HD12	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:NE2	1:A:47:ASN:O	2.44	0.50
2:B:352:LYS:HB3	2:B:376:GLN:OE1	2.12	0.50
2:B:217:LYS:HB3	2:B:339:TRP:HE1	1.77	0.50
2:B:273:ARG:HH11	2:B:273:ARG:HA	1.77	0.50
2:B:350:PRO:HD2	2:B:353:ALA:CB	2.42	0.50
2:B:363:GLN:HG2	2:B:363:GLN:O	2.11	0.50
2:B:402:ILE:HG22	2:B:403:PRO:HD2	1.93	0.50
2:B:273:ARG:NH1	2:B:273:ARG:HA	2.26	0.49
2:B:215:PRO:HB2	2:B:332:LEU:HD22	1.94	0.49
2:B:203:PRO:CB	2:B:204:PRO:HD3	2.38	0.49
2:B:309:LEU:HD13	2:B:382:VAL:HG11	1.94	0.49
2:B:273:ARG:CZ	2:B:273:ARG:HB3	2.42	0.49
2:B:312:GLU:HB3	2:B:324:TRP:HB3	1.95	0.49
1:A:120:ARG:O	1:A:123:THR:HB	2.13	0.49
1:A:145:LYS:HZ3	1:A:146:PHE:HE1	1.60	0.49
2:B:282:THR:HG22	2:B:288:SER:CB	2.43	0.49
2:B:320:LYS:HD2	2:B:321:PRO:HD2	1.94	0.49
1:A:46:GLN:NE2	1:A:50:THR:H	2.10	0.49
2:B:251:CYS:HB3	2:B:254:TYR:CZ	2.48	0.49
2:B:322:TYR:CD1	2:B:322:TYR:C	2.86	0.49
2:B:333:ILE:HG23	2:B:340:PHE:CD2	2.48	0.49
2:B:373:HIS:CE1	2:B:378:TYR:OH	2.65	0.49
1:A:88:GLU:CB	1:A:89:PRO:HD3	2.32	0.48
2:B:322:TYR:CB	2:B:370:LEU:HD23	2.43	0.48
1:A:44:PHE:CD1	1:A:44:PHE:C	2.86	0.48
1:A:44:PHE:CE1	1:A:45:LEU:HD12	2.48	0.48
1:A:123:THR:O	1:A:124:LEU:C	2.51	0.48
2:B:206:LYS:H	2:B:207:PRO:HD2	1.79	0.48
2:B:217:LYS:HE3	2:B:339:TRP:CD1	2.49	0.48
1:A:63:ASN:C	1:A:63:ASN:OD1	2.52	0.48
2:B:282:THR:HG22	2:B:288:SER:HB2	1.96	0.48
2:B:384:CYS:H	2:B:392:SER:HG	1.61	0.48
1:A:44:PHE:CE1	1:A:45:LEU:HB2	2.49	0.48
2:B:211:LYS:HG3	2:B:223:TRP:CE3	2.48	0.47
1:A:77:ARG:NH2	1:A:138:ILE:O	2.47	0.47
1:A:87:LEU:HD22	1:A:111:TYR:HE1	1.79	0.47
2:B:327:TRP:CE2	2:B:365:THR:HA	2.49	0.47
2:B:287:SER:HG	2:B:289:PHE:HE2	1.59	0.47
2:B:347:ARG:HG3	2:B:381:GLN:HG3	1.97	0.47
2:B:313:VAL:HG11	2:B:403:PRO:HD3	1.97	0.47
2:B:303:PRO:HG3	2:B:386:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HA	1:A:81:LEU:HD12	1.96	0.46
1:A:90:VAL:HG11	1:A:114:LEU:CD1	2.45	0.46
1:A:41:LYS:HE3	2:B:294:TYR:OH	2.16	0.46
2:B:402:ILE:CG2	2:B:403:PRO:HD2	2.46	0.46
1:A:40:GLN:O	1:A:41:LYS:C	2.54	0.46
2:B:206:LYS:HD2	2:B:289:PHE:CD2	2.50	0.46
1:A:48:PRO:O	1:A:49:GLN:C	2.55	0.45
1:A:77:ARG:O	1:A:81:LEU:HG	2.16	0.45
2:B:282:THR:HG22	2:B:288:SER:CA	2.45	0.45
1:A:44:PHE:O	1:A:51:SER:HA	2.17	0.45
2:B:287:SER:OG	2:B:289:PHE:HE2	2.00	0.45
2:B:309:LEU:HD11	2:B:325:ILE:CG2	2.47	0.45
1:A:73:LEU:HA	1:A:73:LEU:HD12	1.83	0.45
2:B:242:ARG:HG3	2:B:242:ARG:HH11	1.81	0.45
2:B:257:GLY:HA3	2:B:261:SER:OG	2.17	0.45
1:A:14:MET:HG2	1:A:181:GLN:HE22	1.82	0.45
2:B:322:TYR:CD1	2:B:322:TYR:O	2.70	0.45
2:B:310:ALA:HB3	2:B:326:LYS:HG3	1.99	0.45
2:B:251:CYS:HA	2:B:252:PRO:HD3	1.77	0.45
2:B:238:LEU:HD23	2:B:279:VAL:HG22	1.99	0.45
2:B:324:TRP:O	2:B:326:LYS:NZ	2.50	0.45
1:A:93:LEU:HB3	1:A:97:PHE:CE2	2.51	0.45
2:B:309:LEU:HD11	2:B:325:ILE:HG21	1.98	0.45
1:A:63:ASN:OD1	1:A:66:GLU:HG2	2.18	0.44
1:A:90:VAL:HA	1:A:93:LEU:HB2	1.99	0.44
1:A:72:ASN:CG	1:A:180:VAL:HG13	2.38	0.44
2:B:347:ARG:HD2	2:B:347:ARG:HH11	1.41	0.44
1:A:63:ASN:CG	1:A:66:GLU:HG2	2.38	0.44
1:A:118:GLU:O	1:A:122:GLN:HG3	2.17	0.44
1:A:166:PHE:O	1:A:170:MET:N	2.45	0.44
1:A:45:LEU:HD23	1:A:45:LEU:O	2.18	0.44
1:A:61:PRO:HB2	1:A:67:THR:OG1	2.17	0.44
2:B:225:ARG:HA	2:B:226:PRO:HD3	1.68	0.44
2:B:243:GLU:HB2	2:B:274:THR:H	1.83	0.44
2:B:323:LEU:HA	2:B:323:LEU:HD23	1.74	0.43
1:A:19:ARG:HH22	1:A:104:GLY:CA	2.19	0.43
1:A:77:ARG:CZ	1:A:138:ILE:O	2.66	0.43
2:B:219:THR:HG23	2:B:263:HIS:CE1	2.53	0.43
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.55	0.43
1:A:47:ASN:O	1:A:48:PRO:C	2.57	0.43
2:B:352:LYS:HG3	2:B:353:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:O	1:A:118:GLU:HB2	2.18	0.43
1:A:6:LEU:O	1:A:7:SER:C	2.56	0.43
1:A:23:LEU:HD12	1:A:23:LEU:O	2.18	0.43
2:B:305:PRO:HA	2:B:306:PRO:HD3	1.77	0.43
1:A:76:LEU:CD1	1:A:125:MET:HA	2.48	0.42
2:B:309:LEU:HD13	2:B:382:VAL:CG1	2.48	0.42
2:B:309:LEU:HD22	2:B:382:VAL:HG12	2.00	0.42
2:B:347:ARG:HD3	2:B:394:TRP:CZ2	2.55	0.42
1:A:36:ILE:N	1:A:37:PRO:CD	2.80	0.42
1:A:80:LEU:O	1:A:81:LEU:C	2.58	0.42
2:B:210:PHE:CD1	2:B:225:ARG:HB2	2.55	0.42
2:B:321:PRO:HG2	2:B:372:LEU:O	2.19	0.42
1:A:135:THR:HA	1:A:139:PHE:CE1	2.40	0.42
1:A:46:GLN:HE22	1:A:50:THR:H	1.66	0.42
2:B:347:ARG:HD3	2:B:394:TRP:CD2	2.55	0.42
1:A:178:ARG:HA	1:A:178:ARG:HD2	1.79	0.42
2:B:317:GLU:HG2	2:B:318:ASP:OD2	2.19	0.42
2:B:350:PRO:HB3	2:B:378:TYR:CE2	2.54	0.42
2:B:301:VAL:O	2:B:390:TYR:HB2	2.20	0.42
2:B:385:LYS:HB3	2:B:391:TRP:CE3	2.55	0.42
2:B:217:LYS:HG3	2:B:301:VAL:HG21	2.02	0.41
2:B:217:LYS:HE3	2:B:339:TRP:NE1	2.35	0.41
1:A:97:PHE:O	1:A:105:ALA:HB1	2.20	0.41
1:A:76:LEU:HD13	1:A:125:MET:CA	2.50	0.41
2:B:321:PRO:O	2:B:372:LEU:HB2	2.20	0.41
1:A:78:ILE:HG22	1:A:82:LEU:HD11	2.03	0.41
1:A:27:THR:HG22	1:A:28:TYR:N	2.36	0.41
1:A:20:LEU:HD21	1:A:113:LEU:CB	2.50	0.41
1:A:24:ALA:HB2	1:A:166:PHE:CD2	2.55	0.41
1:A:36:ILE:HG22	1:A:36:ILE:O	2.21	0.41
2:B:213:ARG:HA	2:B:300:ILE:O	2.20	0.41
2:B:307:LEU:O	2:B:328:SER:OG	2.36	0.41
2:B:327:TRP:CH2	2:B:346:ILE:HD11	2.55	0.41
2:B:322:TYR:CD1	2:B:323:LEU:O	2.72	0.41
1:A:19:ARG:HA	1:A:19:ARG:HD2	1.83	0.41
1:A:1:PHE:HA	1:A:2:PRO:HD3	1.69	0.41
1:A:42:TYR:CD2	1:A:45:LEU:HD13	2.54	0.41
1:A:146:PHE:H	1:A:146:PHE:HD1	1.69	0.40
1:A:59:PRO:O	1:A:137:GLN:NE2	2.54	0.40
2:B:342:LEU:O	2:B:343:LEU:HD12	2.21	0.40
2:B:383:ARG:HB3	2:B:394:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:SER:OG	1:A:52:LEU:N	2.53	0.40
2:B:327:TRP:NE1	2:B:365:THR:HA	2.36	0.40
1:A:46:GLN:NE2	1:A:50:THR:HG23	2.36	0.40
2:B:374:PRO:CA	2:B:403:PRO:O	2.69	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	182/191 (95%)	134 (74%)	34 (19%)	14 (8%)	1	3
2	B	191/211 (90%)	150 (78%)	25 (13%)	16 (8%)	1	2
All	All	373/402 (93%)	284 (76%)	59 (16%)	30 (8%)	1	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	49	GLN
2	B	204	PRO
2	B	245	GLU
2	B	246	THR
2	B	317	GLU
2	B	338	GLY
2	B	353	ALA
1	A	141	GLN
1	A	186	GLU
2	B	256	THR
1	A	3	THR
1	A	46	GLN
1	A	48	PRO

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Mol	Chain	Res	Type
1	A	105	ALA
1	A	188	SER
2	B	216	ASN
2	B	257	GLY
2	B	319	ARG
2	B	351	GLU
1	A	65	GLU
2	B	206	LYS
2	B	403	PRO
1	A	64	ARG
1	A	110	VAL
2	B	332	LEU
2	B	387	ASP
2	B	203	PRO
1	A	96	VAL
1	A	4	ILE

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	168/177 (95%)	125 (74%)	43 (26%)	0	2
2	B	176/191 (92%)	142 (81%)	34 (19%)	1	5
All	All	344/368 (94%)	267 (78%)	77 (22%)	1	3

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	LEU
1	A	9	LEU
1	A	12	ASN
1	A	15	LEU
1	A	16	ARG
1	A	20	LEU

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Mol	Chain	Res	Type
1	A	21	HIS
1	A	27	THR
1	A	32	GLU
1	A	35	TYR
1	A	39	GLU
1	A	46	GLN
1	A	47	ASN
1	A	48	PRO
1	A	49	GLN
1	A	51	SER
1	A	52	LEU
1	A	55	SER
1	A	56	GLU
1	A	58	ILE
1	A	71	SER
1	A	74	GLU
1	A	79	SER
1	A	90	VAL
1	A	92	PHE
1	A	95	SER
1	A	103	TYR
1	A	106	SER
1	A	115	LYS
1	A	116	ASP
1	A	118	GLU
1	A	127	ARG
1	A	134	ARG
1	A	143	TYR
1	A	146	PHE
1	A	153	ASP
1	A	157	LEU
1	A	168	LYS
1	A	177	LEU
1	A	179	ILE
1	A	180	VAL
1	A	184	SER
2	B	207	PRO
2	B	228	THR
2	B	229	ASP
2	B	238	LEU
2	B	242	ARG
2	B	267	GLN

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Mol	Chain	Res	Type
2	B	270	SER
2	B	273	ARG
2	B	283	ASN
2	B	288	SER
2	B	300	ILE
2	B	307	LEU
2	B	314	LYS
2	B	315	GLN
2	B	320	LYS
2	B	322	TYR
2	B	325	ILE
2	B	331	THR
2	B	334	ASP
2	B	335	LEU
2	B	343	LEU
2	B	348	LEU
2	B	349	LYS
2	B	352	LYS
2	B	355	GLU
2	B	358	ILE
2	B	364	GLN
2	B	374	PRO
2	B	376	GLN
2	B	381	GLN
2	B	383	ARG
2	B	396	PRO
2	B	399	PHE
2	B	402	ILE

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	12	ASN
1	A	46	GLN
1	A	68	GLN
1	A	122	GLN
1	A	159	ASN
1	A	181	GLN
2	B	241	HIS
2	B	260	ASN
2	B	263	HIS
2	B	267	GLN

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Mol	Chain	Res	Type
2	B	283	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.