



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1GCS / pdb_00001gcs
Title : STRUCTURE OF THE BOVINE GAMMA-B CRYSTALLIN AT 150K
Authors : Najmudin, S.; Lindley, P.; Slingsby, C.; Bateman, O.; Myles, D.; Kumaraswamy, S.; Glover, I.
Deposited on : 1994-01-27
Resolution : 2.00 Å(reported)

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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

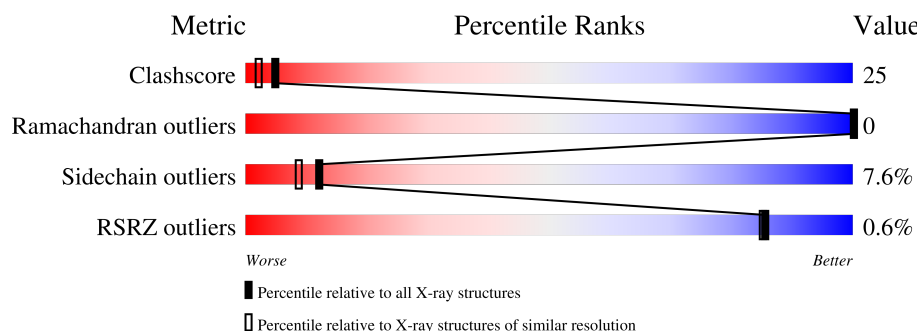
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	174	37% 37% 21% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1729 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 GAMMA-B CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1474	926	266	268	14			

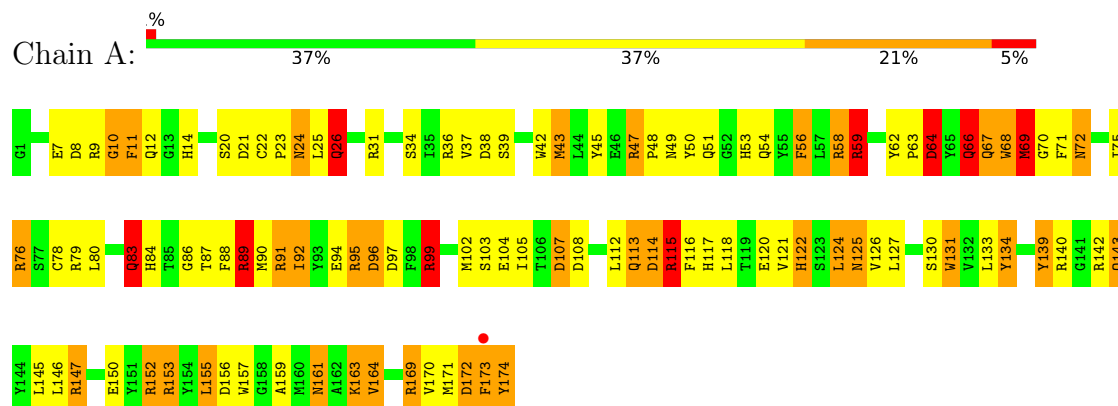
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	255	Total	O	0	0
			255	255		

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 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: GAMMA-B CRYSTALLIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	56.41Å 56.41Å 97.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (8.00-2.00) 92.6 (8.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.48 (at 1.95Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.170 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1729	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.47% 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	1.98	42/1518 (2.8%)	2.47	115/2046 (5.6%)

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	13

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	HIS	CE1-NE2	8.72	1.41	1.32
1	A	14	HIS	ND1-CE1	8.64	1.41	1.32
1	A	62	TYR	CA-CB	-8.63	1.42	1.53
1	A	125	ASN	N-CA	8.61	1.56	1.46
1	A	80	LEU	CA-CB	-8.16	1.42	1.52
1	A	76	ARG	CA-C	-7.86	1.42	1.52
1	A	14	HIS	CE1-NE2	7.26	1.39	1.32
1	A	117	HIS	ND1-CE1	7.20	1.39	1.32
1	A	122	HIS	CE1-NE2	6.94	1.39	1.32
1	A	126	VAL	N-CA	6.92	1.54	1.46
1	A	34	SER	N-CA	6.81	1.54	1.46
1	A	54	GLN	CD-OE1	6.57	1.36	1.23
1	A	64	ASP	CA-CB	-6.54	1.42	1.53
1	A	68	TRP	NE1-CE2	-6.51	1.30	1.37
1	A	56	PHE	N-CA	6.39	1.54	1.46
1	A	88	PHE	N-CA	6.35	1.53	1.46
1	A	117	HIS	CE1-NE2	6.30	1.38	1.32
1	A	83	GLN	CD-OE1	6.20	1.35	1.23
1	A	125	ASN	CG-OD1	6.03	1.35	1.23
1	A	53	HIS	CA-CB	5.95	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLN	CA-C	-5.92	1.45	1.52
1	A	67	GLN	CD-OE1	5.89	1.34	1.23
1	A	14	HIS	CG-CD2	5.82	1.42	1.35
1	A	51	GLN	CD-OE1	5.81	1.34	1.23
1	A	131	TRP	N-CA	5.81	1.53	1.45
1	A	84	HIS	CG-ND1	5.73	1.44	1.38
1	A	59	ARG	CD-NE	-5.66	1.38	1.46
1	A	174	TYR	C-OXT	5.64	1.34	1.23
1	A	22	CYS	C-O	-5.61	1.19	1.24
1	A	127	LEU	N-CA	5.56	1.53	1.46
1	A	24	ASN	CG-OD1	5.48	1.33	1.23
1	A	72	ASN	CG-OD1	5.47	1.33	1.23
1	A	143	GLN	CD-OE1	5.42	1.33	1.23
1	A	84	HIS	ND1-CE1	5.41	1.38	1.32
1	A	173	PHE	N-CA	5.40	1.53	1.46
1	A	26	GLN	CD-OE1	5.37	1.33	1.23
1	A	122	HIS	ND1-CE1	5.34	1.37	1.32
1	A	164	VAL	N-CA	5.28	1.54	1.46
1	A	159	ALA	N-CA	5.26	1.52	1.45
1	A	92	ILE	CA-CB	-5.24	1.47	1.54
1	A	117	HIS	CB-CG	5.13	1.57	1.50
1	A	66	GLN	CD-OE1	5.08	1.33	1.23

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	PHE	CA-CB-CG	-10.87	102.93	113.80
1	A	59	ARG	CD-NE-CZ	10.85	139.59	124.40
1	A	124	LEU	CA-C-N	-10.80	107.77	122.99
1	A	124	LEU	C-N-CA	-10.80	107.77	122.99
1	A	89	ARG	CD-NE-CZ	-10.29	109.99	124.40
1	A	21	ASP	CA-CB-CG	-9.81	102.79	112.60
1	A	64	ASP	CA-CB-CG	9.75	122.35	112.60
1	A	169	ARG	CA-C-N	-8.33	112.07	122.48
1	A	169	ARG	C-N-CA	-8.33	112.07	122.48
1	A	10	GLY	CA-C-N	8.25	133.86	122.07
1	A	10	GLY	C-N-CA	8.25	133.86	122.07
1	A	150	GLU	CA-C-O	8.14	129.74	120.54
1	A	76	ARG	N-CA-C	7.89	123.08	113.38
1	A	150	GLU	O-C-N	-7.83	114.30	123.22
1	A	49	ASN	CA-CB-CG	-7.76	104.84	112.60
1	A	14	HIS	CB-CG-CD2	-7.71	121.18	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	HIS	CA-CB-CG	-7.63	106.17	113.80
1	A	108	ASP	CA-C-O	-7.57	113.31	121.56
1	A	94	GLU	CB-CG-CD	-7.50	99.86	112.60
1	A	75	ILE	CA-C-O	-7.43	111.50	120.78
1	A	64	ASP	CA-C-O	-7.40	113.34	121.33
1	A	94	GLU	O-C-N	7.29	130.47	122.15
1	A	114	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	117	HIS	CA-C-N	7.22	133.16	122.99
1	A	117	HIS	C-N-CA	7.22	133.16	122.99
1	A	12	GLN	OE1-CD-NE2	-7.13	115.47	122.60
1	A	164	VAL	CA-CB-CG1	7.12	122.50	110.40
1	A	107	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	142	ARG	CD-NE-CZ	6.97	134.15	124.40
1	A	125	ASN	CA-C-N	-6.96	113.39	122.37
1	A	125	ASN	C-N-CA	-6.96	113.39	122.37
1	A	67	GLN	OE1-CD-NE2	-6.78	115.82	122.60
1	A	39	SER	CA-C-N	6.69	131.76	122.06
1	A	39	SER	C-N-CA	6.69	131.76	122.06
1	A	95	ARG	O-C-N	-6.69	114.73	123.16
1	A	75	ILE	O-C-N	6.60	130.82	122.57
1	A	50	TYR	O-C-N	-6.54	115.27	122.67
1	A	14	HIS	CA-C-O	6.50	128.30	121.15
1	A	97	ASP	CA-CB-CG	-6.49	106.11	112.60
1	A	94	GLU	CA-C-O	-6.49	113.54	120.42
1	A	79	ARG	CD-NE-CZ	-6.39	115.45	124.40
1	A	134	TYR	CA-C-N	6.39	128.84	120.28
1	A	134	TYR	C-N-CA	6.39	128.84	120.28
1	A	53	HIS	CA-CB-CG	-6.37	107.43	113.80
1	A	8	ASP	CA-C-N	6.32	130.85	120.94
1	A	8	ASP	C-N-CA	6.32	130.85	120.94
1	A	125	ASN	O-C-N	-6.28	115.83	123.30
1	A	157	TRP	CA-C-N	6.26	132.49	120.66
1	A	157	TRP	C-N-CA	6.26	132.49	120.66
1	A	139	TYR	CA-C-N	6.24	134.21	123.03
1	A	139	TYR	C-N-CA	6.24	134.21	123.03
1	A	142	ARG	NE-CZ-NH1	6.23	127.73	121.50
1	A	126	VAL	N-CA-CB	-6.22	103.94	110.72
1	A	14	HIS	CB-CG-ND1	6.17	131.95	122.70
1	A	161	ASN	CA-C-O	-6.16	114.85	121.38
1	A	115	ARG	N-CA-CB	-6.13	101.13	110.33
1	A	172	ASP	CA-C-N	-6.11	110.52	120.72
1	A	172	ASP	C-N-CA	-6.11	110.52	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	37	VAL	CA-CB-CG1	-6.02	100.16	110.40
1	A	112	LEU	CA-C-O	6.00	126.87	119.97
1	A	156	ASP	CA-C-O	-5.98	113.34	120.10
1	A	86	GLY	CA-C-N	5.92	129.76	121.24
1	A	86	GLY	C-N-CA	5.92	129.76	121.24
1	A	76	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	163	LYS	CA-C-N	-5.90	114.97	123.11
1	A	163	LYS	C-N-CA	-5.90	114.97	123.11
1	A	89	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	A	140	ARG	CA-C-O	-5.86	114.77	121.68
1	A	95	ARG	N-CA-C	5.79	119.16	109.95
1	A	45	TYR	CA-C-N	5.77	128.59	120.28
1	A	45	TYR	C-N-CA	5.77	128.59	120.28
1	A	87	THR	N-CA-C	5.77	118.07	109.59
1	A	96	ASP	O-C-N	-5.76	115.62	122.65
1	A	170	VAL	CA-CB-CG2	5.70	120.08	110.40
1	A	96	ASP	CA-C-O	5.67	128.46	121.99
1	A	150	GLU	CA-C-N	-5.66	114.05	123.33
1	A	150	GLU	C-N-CA	-5.66	114.05	123.33
1	A	7	GLU	CA-CB-CG	-5.66	102.79	114.10
1	A	37	VAL	O-C-N	5.64	129.76	122.77
1	A	37	VAL	CA-C-O	-5.63	113.88	120.75
1	A	134	TYR	CA-C-O	5.55	126.36	120.36
1	A	58	ARG	CD-NE-CZ	-5.54	116.64	124.40
1	A	122	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	169	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	A	108	ASP	O-C-N	5.50	129.34	122.86
1	A	172	ASP	O-C-N	-5.46	115.05	122.36
1	A	71	PHE	CA-C-O	5.45	125.65	119.27
1	A	140	ARG	CA-C-N	5.42	139.60	120.73
1	A	140	ARG	C-N-CA	5.42	139.60	120.73
1	A	69	MET	N-CA-C	-5.41	105.44	113.40
1	A	147	ARG	CD-NE-CZ	5.41	131.98	124.40
1	A	79	ARG	CG-CD-NE	-5.40	100.11	112.00
1	A	108	ASP	N-CA-C	-5.38	102.91	110.50
1	A	76	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	42	TRP	CA-C-N	5.37	130.73	123.11
1	A	42	TRP	C-N-CA	5.37	130.73	123.11
1	A	70	GLY	CA-C-O	5.31	127.63	121.90
1	A	12	GLN	CG-CD-NE2	5.27	124.31	116.40
1	A	125	ASN	N-CA-CB	-5.27	101.82	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	157	TRP	CA-CB-CG	5.22	123.53	113.60
1	A	36	ARG	CD-NE-CZ	-5.22	117.10	124.40
1	A	38	ASP	N-CA-C	-5.19	106.10	112.90
1	A	130	SER	CA-C-N	-5.15	114.16	122.82
1	A	130	SER	C-N-CA	-5.15	114.16	122.82
1	A	89	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	A	20	SER	CA-C-N	-5.11	112.24	120.87
1	A	20	SER	C-N-CA	-5.11	112.24	120.87
1	A	23	PRO	O-C-N	-5.09	115.22	122.35
1	A	78	CYS	O-C-N	5.08	129.07	123.33
1	A	53	HIS	CB-CA-C	-5.08	100.19	109.54
1	A	142	ARG	N-CA-C	5.02	117.58	110.10
1	A	36	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	43	MET	N-CA-CB	5.01	118.78	110.47

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	147	ARG	Sidechain
1	A	152	ARG	Sidechain
1	A	153	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	31	ARG	Sidechain
1	A	47	ARG	Sidechain
1	A	59	ARG	Sidechain
1	A	76	ARG	Sidechain
1	A	89	ARG	Sidechain
1	A	9	ARG	Sidechain
1	A	91	ARG	Sidechain
1	A	99	ARG	Sidechain

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	1370	72	0
2	A	255	0	0	29	4
All	All	1729	0	1370	72	4

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 25.

All (72) 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:68:TRP:O	1:A:69:MET:HB2	1.49	1.10
1:A:67:GLN:HG3	2:A:402:HOH:O	1.53	1.09
1:A:96:ASP:HB3	2:A:287:HOH:O	1.65	0.97
1:A:173:PHE:HZ	2:A:441:HOH:O	1.50	0.92
1:A:58:ARG:NH1	2:A:434:HOH:O	2.08	0.86
1:A:69:MET:HB3	2:A:328:HOH:O	1.77	0.85
1:A:89:ARG:NH1	1:A:104:GLU:OE2	2.11	0.83
1:A:69:MET:HA	1:A:69:MET:HE3	1.63	0.80
1:A:113:GLN:NE2	2:A:282:HOH:O	2.14	0.80
1:A:59:ARG:NH1	1:A:173:PHE:CD1	2.51	0.79
1:A:56:PHE:H	1:A:143:GLN:HE22	1.31	0.79
1:A:83:GLN:HG2	2:A:377:HOH:O	1.82	0.78
1:A:68:TRP:O	1:A:69:MET:CB	2.26	0.77
1:A:89:ARG:HD2	1:A:104:GLU:CD	2.09	0.76
1:A:83:GLN:CG	2:A:377:HOH:O	2.34	0.73
1:A:59:ARG:HH12	1:A:173:PHE:HB2	1.56	0.70
1:A:152:ARG:HG2	2:A:383:HOH:O	1.94	0.67
1:A:116:PHE:HB3	1:A:118:LEU:HD12	1.76	0.66
1:A:173:PHE:C	1:A:174:TYR:CD1	2.75	0.65
1:A:114:ASP:OD1	2:A:426:HOH:O	2.14	0.64
1:A:83:GLN:O	2:A:272:HOH:O	2.15	0.63
1:A:26:GLN:OE1	1:A:48:PRO:HG3	1.99	0.62
1:A:122:HIS:HB3	2:A:287:HOH:O	1.99	0.62
1:A:122:HIS:HD2	2:A:335:HOH:O	1.81	0.62
1:A:59:ARG:NH1	1:A:173:PHE:HD1	1.97	0.59
1:A:66:GLN:OE1	2:A:413:HOH:O	2.17	0.59
1:A:172:ASP:HB3	1:A:174:TYR:O	2.02	0.59
1:A:116:PHE:CB	1:A:118:LEU:HD12	2.34	0.56
1:A:69:MET:HA	1:A:69:MET:CE	2.35	0.56
1:A:24:ASN:OD1	1:A:26:GLN:HG3	2.05	0.55
1:A:69:MET:HE1	2:A:236:HOH:O	2.05	0.55
1:A:171:MET:HG2	2:A:330:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:CD2	2:A:335:HOH:O	2.58	0.53
1:A:89:ARG:HG3	1:A:90:MET:N	2.24	0.52
1:A:173:PHE:C	1:A:174:TYR:HD1	2.16	0.52
1:A:155:LEU:HD12	2:A:386:HOH:O	2.09	0.51
1:A:43:MET:HG2	1:A:145:LEU:HB2	1.92	0.51
1:A:134:TYR:CG	1:A:139:TYR:HA	2.46	0.51
1:A:173:PHE:HA	2:A:419:HOH:O	2.11	0.51
1:A:120:GLU:OE1	1:A:122:HIS:HE1	1.93	0.50
1:A:72:ASN:HB2	2:A:279:HOH:O	2.11	0.50
1:A:173:PHE:HD2	2:A:439:HOH:O	1.94	0.49
1:A:91:ARG:HD3	1:A:102:MET:SD	2.53	0.49
1:A:58:ARG:NH1	2:A:417:HOH:O	2.45	0.49
1:A:96:ASP:OD2	1:A:153:ARG:NH2	2.47	0.48
1:A:174:TYR:CD1	1:A:174:TYR:N	2.82	0.47
1:A:99:ARG:HE	1:A:99:ARG:HB2	1.32	0.46
1:A:83:GLN:HG3	2:A:377:HOH:O	2.07	0.46
1:A:59:ARG:NH2	1:A:173:PHE:H	2.14	0.46
1:A:92:ILE:O	1:A:102:MET:HA	2.15	0.46
1:A:63:PRO:HD2	2:A:402:HOH:O	2.16	0.45
1:A:47:ARG:HD2	2:A:389:HOH:O	2.17	0.45
1:A:152:ARG:CG	2:A:383:HOH:O	2.60	0.43
1:A:10:GLY:C	1:A:11:PHE:CD2	2.96	0.43
1:A:25:LEU:O	1:A:26:GLN:C	2.61	0.43
1:A:173:PHE:CZ	2:A:441:HOH:O	2.41	0.43
1:A:89:ARG:CD	1:A:104:GLU:CD	2.88	0.42
1:A:125:ASN:C	1:A:125:ASN:HD22	2.26	0.42
1:A:59:ARG:HH12	1:A:173:PHE:CB	2.29	0.42
1:A:90:MET:HG2	1:A:131:TRP:CZ2	2.55	0.41
1:A:124:LEU:C	1:A:124:LEU:HD12	2.45	0.41
1:A:161:ASN:OD1	1:A:163:LYS:HB2	2.20	0.41
1:A:92:ILE:HG12	1:A:105:ILE:HD12	2.02	0.41
1:A:47:ARG:HG2	2:A:389:HOH:O	2.21	0.41
1:A:121:VAL:HB	1:A:164:VAL:HG21	2.02	0.41
1:A:64:ASP:OD1	1:A:66:GLN:HB2	2.21	0.41
1:A:153:ARG:C	1:A:155:LEU:N	2.79	0.40
1:A:59:ARG:HH22	1:A:173:PHE:H	1.68	0.40
1:A:59:ARG:CZ	1:A:173:PHE:HD1	2.33	0.40
1:A:95:ARG:HB2	1:A:99:ARG:HB3	2.02	0.40
1:A:115:ARG:NH2	2:A:423:HOH:O	2.50	0.40
1:A:133:LEU:HB2	1:A:146:LEU:HD11	2.02	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:452:HOH:O	2:A:452:HOH:O[8_555]	1.61	0.59
2:A:255:HOH:O	2:A:255:HOH:O[7_556]	1.82	0.38
2:A:304:HOH:O	2:A:389:HOH:O[4_454]	1.87	0.33
2:A:303:HOH:O	2:A:375:HOH:O[4_454]	2.07	0.13

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	172/174 (99%)	167 (97%)	5 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	158/158 (100%)	146 (92%)	12 (8%)	12	9

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	59	ARG
1	A	64	ASP

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Mol	Chain	Res	Type
1	A	66	GLN
1	A	69	MET
1	A	83	GLN
1	A	99	ARG
1	A	103	SER
1	A	107	ASP
1	A	113	GLN
1	A	115	ARG
1	A	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	66	GLN
1	A	67	GLN
1	A	83	GLN
1	A	113	GLN
1	A	122	HIS
1	A	125	ASN
1	A	143	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	174/174 (100%)	-0.61	1 (0%) 85 85	3, 10, 28, 41	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	PHE	3.8

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.