



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:27 PM UTC

PDB ID : 7VPS / pdb_00007vps
Title : Crystal structure of the ARM domain of C. glabrata importin alpha
Authors : Tan, L.; Im, Y.J.
Deposited on : 2021-10-17
Resolution : 2.29 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

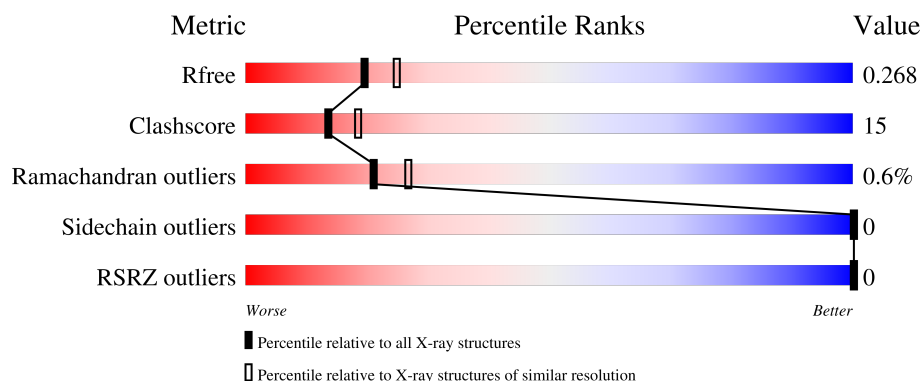
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	447	 66% 30% ..
1	B	447	 72% 23% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7105 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 Importin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3398	2143	573	665	17			
1	B	438	Total	C	N	O	S	0	0	0
			3392	2140	572	663	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP Q6FNI4
A	71	SER	-	expression tag	UNP Q6FNI4
A	72	ALA	-	expression tag	UNP Q6FNI4
A	73	MET	-	expression tag	UNP Q6FNI4
A	74	GLY	-	expression tag	UNP Q6FNI4
B	70	GLY	-	expression tag	UNP Q6FNI4
B	71	SER	-	expression tag	UNP Q6FNI4
B	72	ALA	-	expression tag	UNP Q6FNI4
B	73	MET	-	expression tag	UNP Q6FNI4
B	74	GLY	-	expression tag	UNP Q6FNI4

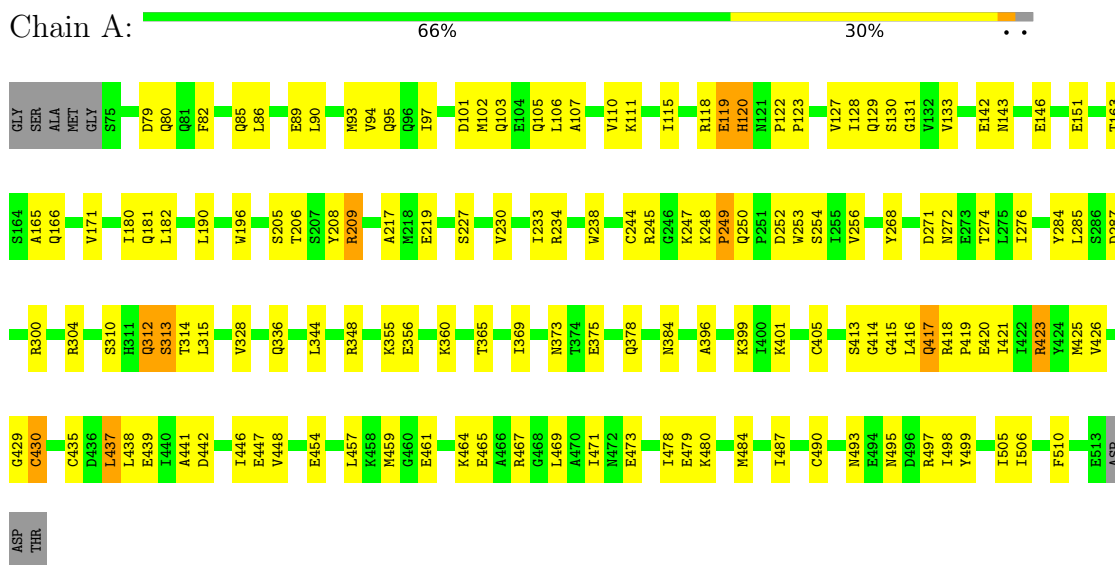
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	153	Total	O	0	0
			153	153		
2	B	162	Total	O	0	0
			162	162		

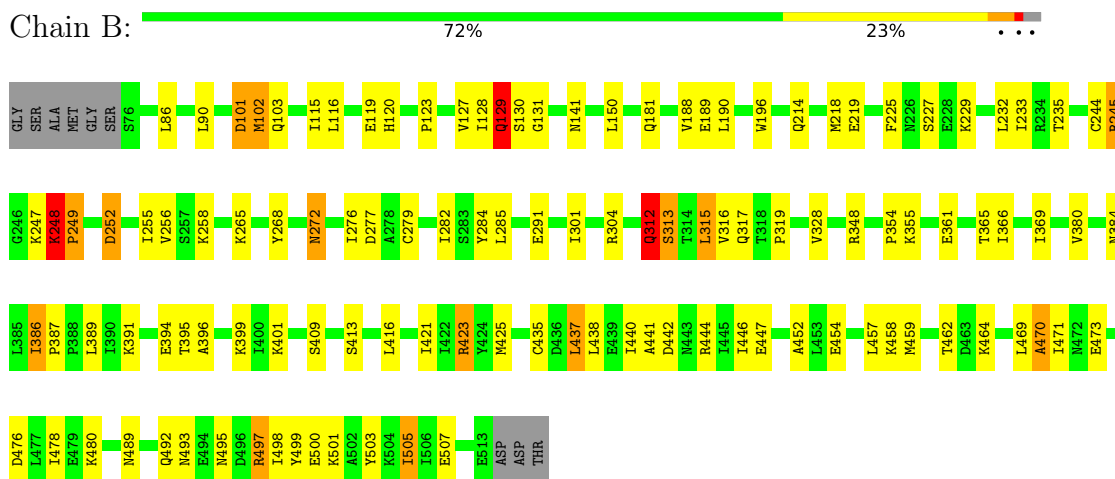
3 Residue-property plots

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: Importin subunit alpha



• Molecule 1: Importin subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.65Å 62.63Å 154.65Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	31.31 – 2.29 31.31 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.7 (31.31-2.29) 96.6 (31.31-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.218 , 0.267 0.218 , 0.268	Depositor DCC
R_{free} test set	2008 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 15.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7105	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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	0.68	10/3451 (0.3%)	1.02	17/4693 (0.4%)
1	B	0.60	3/3445 (0.1%)	0.99	30/4685 (0.6%)
All	All	0.64	13/6896 (0.2%)	1.00	47/9378 (0.5%)

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	5
1	B	0	6
All	All	0	11

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	386	ILE	C-O	8.77	1.32	1.24
1	A	122	PRO	C-O	-6.91	1.16	1.24
1	B	423	ARG	CZ-NH2	-6.69	1.24	1.33
1	A	120	HIS	C-O	-6.63	1.15	1.24
1	A	356	GLU	C-O	-6.31	1.16	1.24
1	A	415	GLY	C-O	-6.16	1.15	1.23
1	A	413	SER	CA-C	-6.15	1.44	1.52
1	A	105	GLN	C-O	-5.71	1.17	1.24
1	B	249	PRO	C-O	-5.64	1.17	1.23
1	A	413	SER	C-O	-5.28	1.17	1.23
1	A	133	VAL	CA-CB	-5.23	1.51	1.54
1	A	103	GLN	C-O	-5.21	1.17	1.24
1	A	106	LEU	C-O	-5.04	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	GLY	N-CA-C	-12.90	95.87	111.35
1	A	423	ARG	CG-CD-NE	-10.40	89.11	112.00
1	B	248	LYS	N-CA-C	-8.81	90.33	109.81
1	B	423	ARG	CG-CD-NE	-8.79	92.65	112.00
1	B	128	ILE	CA-C-N	-8.54	108.48	122.65
1	B	128	ILE	C-N-CA	-8.54	108.48	122.65
1	B	497	ARG	CB-CG-CD	-7.94	93.03	111.30
1	B	313	SER	O-C-N	-7.83	114.13	123.13
1	A	429	GLY	CA-C-N	7.78	130.70	120.28
1	A	429	GLY	C-N-CA	7.78	130.70	120.28
1	A	119	GLU	CA-C-N	-7.35	111.92	122.94
1	A	119	GLU	C-N-CA	-7.35	111.92	122.94
1	B	312	GLN	O-C-N	-7.07	112.96	122.43
1	B	312	GLN	CA-C-N	7.02	131.77	122.30
1	B	312	GLN	C-N-CA	7.02	131.77	122.30
1	B	315	LEU	CA-C-N	6.85	130.53	120.74
1	B	315	LEU	C-N-CA	6.85	130.53	120.74
1	B	399	LYS	CB-CG-CD	-6.63	96.06	111.30
1	A	313	SER	O-C-N	-6.59	114.82	122.93
1	A	312	GLN	CA-C-N	6.55	130.12	120.95
1	A	312	GLN	C-N-CA	6.55	130.12	120.95
1	B	249	PRO	N-CA-C	-6.54	100.22	110.50
1	B	247	LYS	N-CA-C	-6.52	97.79	108.41
1	A	128	ILE	CA-C-N	-6.39	109.53	122.31
1	A	128	ILE	C-N-CA	-6.39	109.53	122.31
1	B	101	ASP	CA-C-N	-6.25	110.02	121.52
1	B	101	ASP	C-N-CA	-6.25	110.02	121.52
1	B	386	ILE	O-C-N	-6.19	116.46	120.42
1	A	480	LYS	CA-CB-CG	-6.14	101.82	114.10
1	B	489	ASN	CA-C-N	-5.93	111.64	122.38
1	B	489	ASN	C-N-CA	-5.93	111.64	122.38
1	B	245	ARG	N-CA-C	5.83	118.72	110.50
1	B	497	ARG	CG-CD-NE	5.75	124.65	112.00
1	A	79	ASP	O-C-N	-5.67	115.59	122.22
1	B	102	MET	O-C-N	-5.65	114.33	122.36
1	B	272	ASN	CB-CA-C	5.31	119.88	110.85
1	A	209	ARG	CG-CD-NE	-5.25	100.44	112.00
1	B	248	LYS	CA-C-N	-5.23	113.80	120.23
1	B	248	LYS	C-N-CA	-5.23	113.80	120.23
1	B	129	GLN	CA-C-N	-5.20	112.50	121.66
1	B	129	GLN	C-N-CA	-5.20	112.50	121.66
1	B	227	SER	CA-C-N	-5.15	114.55	123.25
1	B	227	SER	C-N-CA	-5.15	114.55	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	GLN	N-CA-C	5.11	117.24	111.11
1	A	227	SER	CA-C-N	-5.07	114.52	122.79
1	A	227	SER	C-N-CA	-5.07	114.52	122.79
1	B	505	ILE	N-CA-CB	5.02	117.00	110.57

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLN	Mainchain
1	A	248	LYS	Peptide
1	A	430	CYS	Mainchain
1	A	437	LEU	Mainchain
1	A	439	GLU	Mainchain
1	B	129	GLN	Mainchain
1	B	312	GLN	Mainchain
1	B	316	VAL	Mainchain
1	B	437	LEU	Mainchain
1	B	469	LEU	Peptide
1	B	470	ALA	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	3398	0	3427	107	8
1	B	3392	0	3422	93	11
2	A	153	0	0	9	2
2	B	162	0	0	10	3
All	All	7105	0	6849	199	22

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 15.

All (199) 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:465:GLU:OE1	2:A:601:HOH:O	1.59	1.15
1:B:248:LYS:HB3	1:B:249:PRO:CD	1.76	1.15
1:A:378:GLN:OE1	1:A:418:ARG:NH2	1.81	1.11
1:B:459:MET:HE3	1:B:459:MET:HA	1.33	1.10
1:B:248:LYS:HB3	1:B:249:PRO:HD3	1.34	1.06
1:A:495:ASN:HD22	1:A:498:ILE:HG23	1.26	1.00
1:B:248:LYS:CB	1:B:249:PRO:CD	2.39	0.98
1:B:225:PHE:HD1	1:B:233:ILE:HG23	1.29	0.98
1:A:209:ARG:NH1	1:A:245:ARG:O	2.01	0.92
1:B:225:PHE:CD1	1:B:233:ILE:HG23	2.05	0.92
1:A:461:GLU:OE1	1:A:464:LYS:NZ	2.08	0.87
1:A:495:ASN:ND2	1:A:498:ILE:HG23	1.90	0.87
1:B:493:ASN:CB	1:B:498:ILE:HD11	2.07	0.85
1:A:487:ILE:HG21	1:A:505:ILE:HD11	1.60	0.83
1:A:378:GLN:CD	1:A:418:ARG:HH22	1.85	0.83
1:B:248:LYS:CB	1:B:249:PRO:HD2	2.11	0.80
1:A:348:ARG:NH1	1:A:384:ASN:O	2.15	0.80
1:A:435:CYS:HA	1:A:438:LEU:HD23	1.64	0.79
1:A:310:SER:OG	2:A:602:HOH:O	1.86	0.77
1:A:163:THR:HG22	1:A:165:ALA:N	2.00	0.76
1:A:250:GLN:NE2	2:A:603:HOH:O	2.17	0.75
1:B:248:LYS:HB2	2:B:623:HOH:O	1.88	0.73
1:B:141:ASN:ND2	2:B:601:HOH:O	2.03	0.73
1:A:101:ASP:OD1	1:A:102:MET:N	2.23	0.71
1:B:277:ASP:OD2	2:B:603:HOH:O	2.08	0.70
1:A:284:TYR:O	2:A:603:HOH:O	2.09	0.70
1:A:490:CYS:HB3	1:A:498:ILE:HD12	1.72	0.70
1:B:272:ASN:O	1:B:276:ILE:HD12	1.91	0.70
1:B:248:LYS:HB2	1:B:249:PRO:HD2	1.72	0.69
1:B:244:CYS:SG	1:B:285:LEU:HD21	2.33	0.69
1:B:258:LYS:O	2:B:605:HOH:O	2.10	0.69
1:A:182:LEU:HD13	1:A:190:LEU:HD21	1.72	0.69
1:B:119:GLU:O	2:B:604:HOH:O	2.10	0.69
1:A:447:GLU:HG2	1:A:498:ILE:HG22	1.76	0.67
1:B:245:ARG:HG3	1:B:284:TYR:CE2	2.29	0.67
1:B:459:MET:HA	1:B:459:MET:CE	2.20	0.67
1:A:82:PHE:CZ	1:A:118:ARG:HD2	2.30	0.67
1:A:219:GLU:OE1	1:A:219:GLU:HA	1.95	0.66
1:A:312:GLN:NE2	1:A:312:GLN:H	1.93	0.66
1:A:336:GLN:OE1	2:A:606:HOH:O	2.13	0.66
1:B:447:GLU:HG2	1:B:498:ILE:HG22	1.78	0.65
1:B:421:ILE:HG22	1:B:425:MET:HE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HG2	1:A:120:HIS:NE2	2.12	0.65
1:B:413:SER:OG	2:B:602:HOH:O	2.06	0.64
1:A:163:THR:HG22	1:A:165:ALA:H	1.61	0.64
1:B:459:MET:HE3	1:B:459:MET:CA	2.19	0.63
1:A:252:ASP:O	1:A:256:VAL:HG12	1.99	0.62
1:B:493:ASN:HB3	1:B:498:ILE:HD11	1.81	0.62
1:A:426:VAL:HA	1:A:430:CYS:SG	2.40	0.61
1:B:464:LYS:HG3	1:B:470:ALA:HA	1.82	0.61
1:A:419:PRO:HA	1:A:459:MET:HE3	1.82	0.61
1:A:256:VAL:HG22	1:A:285:LEU:HD21	1.82	0.61
1:A:396:ALA:O	1:A:401:LYS:HD2	2.01	0.60
1:B:348:ARG:NH1	1:B:384:ASN:O	2.35	0.60
1:A:268:TYR:CE1	1:A:304:ARG:HD3	2.37	0.59
1:A:416:LEU:HB2	1:A:417:GLN:NE2	2.17	0.59
1:B:361:GLU:OE1	2:B:606:HOH:O	2.17	0.59
1:B:493:ASN:HB2	1:B:498:ILE:HD11	1.85	0.59
1:B:355:LYS:HA	1:B:355:LYS:HE2	1.85	0.58
1:B:369:ILE:HD11	1:B:380:VAL:CG2	2.33	0.58
1:B:435:CYS:HA	1:B:438:LEU:HD23	1.85	0.58
1:B:268:TYR:CE1	1:B:304:ARG:HD3	2.39	0.58
1:B:313:SER:O	1:B:317:GLN:HG3	2.03	0.58
1:B:444:ARG:HD2	1:B:444:ARG:O	2.03	0.58
1:A:119:GLU:HG2	1:A:120:HIS:CD2	2.39	0.57
1:B:457:LEU:HD13	1:B:505:ILE:CG2	2.34	0.57
1:B:366:ILE:HG21	1:B:389:LEU:HD11	1.85	0.57
1:B:219:GLU:HA	1:B:219:GLU:OE2	2.05	0.56
1:A:86:LEU:HD11	1:A:115:ILE:HD12	1.86	0.56
1:A:256:VAL:CG2	1:A:285:LEU:HD21	2.35	0.56
1:B:123:PRO:O	1:B:127:VAL:HG13	2.07	0.55
1:A:405:CYS:SG	1:A:448:VAL:HG23	2.46	0.55
1:A:163:THR:CG2	1:A:165:ALA:H	2.20	0.55
1:A:244:CYS:SG	1:A:256:VAL:HG23	2.46	0.55
1:A:498:ILE:HG13	1:A:499:TYR:N	2.22	0.55
1:B:369:ILE:HD11	1:B:380:VAL:HG22	1.88	0.55
1:A:487:ILE:HD13	1:A:505:ILE:HD11	1.89	0.54
1:A:123:PRO:O	1:A:127:VAL:HG23	2.08	0.54
1:B:396:ALA:O	1:B:401:LYS:HD2	2.08	0.54
1:A:435:CYS:HA	1:A:438:LEU:CD2	2.35	0.54
1:B:188:VAL:HG21	1:B:229:LYS:HG3	1.89	0.54
1:A:209:ARG:NH2	1:A:249:PRO:O	2.34	0.53
1:B:86:LEU:HD11	1:B:115:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HG	1:A:441:ALA:HB2	1.90	0.53
1:B:188:VAL:HG12	1:B:189:GLU:OE1	2.09	0.53
1:A:378:GLN:CG	1:A:418:ARG:HH22	2.21	0.52
1:A:442:ASP:O	1:A:446:ILE:HG12	2.10	0.52
1:A:344:LEU:HD21	1:A:369:ILE:HD11	1.90	0.52
1:A:230:VAL:O	1:A:233:ILE:HG13	2.10	0.52
1:A:93:MET:HE3	1:A:111:LYS:HB2	1.91	0.52
1:A:182:LEU:HB3	1:A:190:LEU:CD2	2.39	0.52
1:B:476:ASP:O	1:B:480:LYS:HG3	2.09	0.52
1:B:245:ARG:HG3	1:B:284:TYR:CZ	2.45	0.52
1:A:446:ILE:HG21	1:A:498:ILE:HD13	1.93	0.51
1:A:461:GLU:CD	1:A:464:LYS:HZ3	2.09	0.51
1:A:493:ASN:CB	1:A:498:ILE:HD11	2.41	0.51
1:B:291:GLU:CD	1:B:291:GLU:H	2.19	0.51
1:B:492:GLN:OE1	2:B:607:HOH:O	2.18	0.51
1:B:282:ILE:HD13	1:B:301:ILE:HG21	1.93	0.50
1:A:111:LYS:O	1:A:115:ILE:HG23	2.11	0.50
1:A:360:LYS:HD2	1:A:399:LYS:HE3	1.94	0.50
1:A:479:GLU:HG2	1:A:484:MET:SD	2.52	0.50
1:A:107:ALA:O	1:A:111:LYS:HG3	2.12	0.50
1:A:146:GLU:OE2	2:A:607:HOH:O	2.20	0.50
1:A:180:ILE:HD11	1:A:217:ALA:HB2	1.93	0.50
1:A:205:SER:OG	1:A:208:TYR:N	2.33	0.49
1:A:487:ILE:HG21	1:A:505:ILE:CD1	2.36	0.49
1:A:101:ASP:OD1	1:A:101:ASP:C	2.55	0.49
1:B:102:MET:O	1:B:103:GLN:C	2.52	0.49
1:A:505:ILE:HG13	1:A:506:ILE:N	2.28	0.48
1:B:500:GLU:HA	1:B:503:TYR:HB3	1.94	0.48
1:A:247:LYS:HE2	1:A:287:ASP:OD2	2.13	0.48
1:A:272:ASN:O	1:A:276:ILE:HD12	2.13	0.48
1:B:369:ILE:CD1	1:B:380:VAL:CG2	2.92	0.48
1:B:101:ASP:OD1	1:B:102:MET:N	2.47	0.48
1:B:150:LEU:HA	1:B:190:LEU:HD13	1.96	0.48
1:A:416:LEU:H	1:A:416:LEU:HD22	1.79	0.47
1:A:85:GLN:O	1:A:89:GLU:OE2	2.32	0.47
1:A:467:ARG:HB3	1:A:469:LEU:CD2	2.43	0.47
1:B:498:ILE:HG13	1:B:499:TYR:N	2.29	0.47
1:A:421:ILE:HD11	2:A:635:HOH:O	2.14	0.47
1:A:378:GLN:HB2	1:A:418:ARG:NH2	2.30	0.47
1:B:188:VAL:HG23	1:B:232:LEU:HD22	1.96	0.47
1:B:248:LYS:HB3	1:B:249:PRO:HD2	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:TRP:CZ3	1:A:238:TRP:CZ3	3.01	0.47
1:A:416:LEU:CB	1:A:417:GLN:NE2	2.77	0.47
1:B:279:CYS:HB3	1:B:319:PRO:HB2	1.96	0.47
1:B:386:ILE:HB	1:B:387:PRO:HD3	1.96	0.47
1:B:188:VAL:CG1	1:B:189:GLU:OE1	2.63	0.47
1:A:495:ASN:ND2	1:A:498:ILE:H	2.13	0.47
1:A:467:ARG:NH2	2:A:622:HOH:O	2.45	0.46
1:A:233:ILE:CD1	1:A:274:THR:HG21	2.45	0.46
1:A:313:SER:OG	1:A:315:LEU:HB2	2.15	0.46
1:B:245:ARG:HG3	1:B:284:TYR:CD2	2.50	0.46
1:B:409:SER:HB2	1:B:452:ALA:HB2	1.98	0.46
1:B:459:MET:CE	1:B:462:THR:HB	2.47	0.45
1:A:142:GLU:HG3	1:A:143:ASN:ND2	2.31	0.45
1:B:252:ASP:HB3	1:B:255:ILE:HD12	1.99	0.45
1:B:416:LEU:CD2	1:B:459:MET:HE3	2.47	0.45
1:A:490:CYS:HB3	1:A:498:ILE:CD1	2.44	0.45
1:B:218:MET:HE3	1:B:256:VAL:HA	1.97	0.45
1:A:493:ASN:HB2	1:A:498:ILE:HD11	1.97	0.45
1:B:90:LEU:HD21	1:B:130:SER:HB3	1.99	0.45
1:B:268:TYR:CZ	1:B:304:ARG:HD3	2.52	0.45
1:A:416:LEU:H	1:A:416:LEU:CD2	2.29	0.44
1:A:419:PRO:HA	1:A:459:MET:CE	2.45	0.44
1:B:196:TRP:HB2	1:B:235:THR:HG21	1.99	0.44
1:A:233:ILE:HD12	1:A:274:THR:CG2	2.48	0.44
1:A:244:CYS:SG	1:A:256:VAL:CG2	3.06	0.44
1:B:457:LEU:HD21	1:B:478:ILE:HD12	2.00	0.44
1:A:234:ARG:NH2	1:A:271:ASP:OD2	2.39	0.44
1:B:447:GLU:OE2	1:B:497:ARG:NH2	2.50	0.44
1:B:497:ARG:HH21	1:B:497:ARG:HD2	1.63	0.44
1:A:110:VAL:HG22	1:A:151:GLU:CD	2.42	0.44
1:A:252:ASP:OD1	1:A:254:SER:HB3	2.18	0.44
1:B:464:LYS:CG	1:B:470:ALA:HA	2.47	0.44
1:A:163:THR:HB	1:A:166:GLN:HG3	1.99	0.43
1:B:394:GLU:HG2	1:B:395:THR:CG2	2.48	0.43
1:B:328:VAL:HG21	1:B:365:THR:HG23	1.99	0.43
1:A:454:GLU:OE1	1:A:505:ILE:HG22	2.18	0.43
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.84	0.43
1:A:471:ILE:HD11	1:A:473:GLU:OE1	2.19	0.43
1:B:437:LEU:HD12	1:B:440:ILE:HD11	2.01	0.43
1:A:171:VAL:HG21	1:A:208:TYR:CE2	2.54	0.43
1:B:447:GLU:OE1	1:B:501:LYS:NZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:H	1:A:420:GLU:CD	2.27	0.43
1:B:457:LEU:HD13	1:B:505:ILE:HG23	2.00	0.43
1:A:253:TRP:HA	1:A:256:VAL:CG1	2.49	0.43
1:B:446:ILE:HG21	1:B:498:ILE:HD13	2.00	0.43
1:B:495:ASN:OD1	1:B:498:ILE:HG23	2.19	0.42
1:B:492:GLN:HG3	2:B:737:HOH:O	2.18	0.42
1:A:373:ASN:HB3	1:A:375:GLU:OE2	2.20	0.42
1:B:503:TYR:CE1	1:B:507:GLU:HG3	2.54	0.42
1:A:437:LEU:HG	1:A:437:LEU:O	2.19	0.42
1:B:387:PRO:O	1:B:391:LYS:HE3	2.20	0.42
1:A:181:GLN:NE2	1:B:265:LYS:NZ	2.67	0.42
1:A:82:PHE:CE2	1:A:118:ARG:HD2	2.54	0.41
1:A:90:LEU:HD21	1:A:130:SER:HB3	2.01	0.41
1:A:421:ILE:O	1:A:425:MET:HG3	2.19	0.41
1:B:454:GLU:OE2	1:B:458:LYS:HE3	2.20	0.41
1:B:116:LEU:HD11	1:B:127:VAL:HG21	2.02	0.41
1:A:94:VAL:O	1:A:97:ILE:HG22	2.20	0.41
1:A:506:ILE:HA	1:A:510:PHE:HD2	1.86	0.41
1:B:189:GLU:H	1:B:189:GLU:CD	2.27	0.41
1:B:442:ASP:O	1:B:446:ILE:HG12	2.21	0.41
1:A:457:LEU:HD21	1:A:478:ILE:HD12	2.03	0.41
1:A:312:GLN:N	1:A:312:GLN:CD	2.79	0.41
1:B:354:PRO:O	1:B:355:LYS:HE2	2.21	0.41
1:B:471:ILE:H	1:B:471:ILE:HG13	1.80	0.41
1:A:206:THR:HG21	1:A:249:PRO:HD2	2.02	0.41
1:A:328:VAL:HG21	1:A:365:THR:HG23	2.02	0.41
1:B:437:LEU:HG	1:B:441:ALA:HB2	2.02	0.41
1:B:181:GLN:NE2	2:B:629:HOH:O	2.54	0.40
1:B:313:SER:OG	1:B:315:LEU:HB2	2.21	0.40
1:A:95:GLN:NE2	2:A:625:HOH:O	2.48	0.40
1:B:459:MET:CE	1:B:459:MET:CA	2.91	0.40
1:A:314:THR:HB	1:A:355:LYS:HE2	2.04	0.40
1:B:244:CYS:SG	1:B:285:LEU:CD2	3.07	0.40
1:A:233:ILE:HD12	1:A:274:THR:HG21	2.03	0.40

All (22) 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)
1:B:131:GLY:N	1:B:423:ARG:NH2[1_445]	0.67	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLY:CA	1:B:423:ARG:NH1[1_445]	1.00	1.20
1:B:131:GLY:CA	1:B:423:ARG:CZ[1_445]	1.06	1.14
1:A:131:GLY:CA	1:A:423:ARG:NH2[1_465]	1.10	1.10
1:B:130:SER:C	1:B:423:ARG:NH2[1_445]	1.34	0.86
1:A:131:GLY:N	1:A:423:ARG:NH2[1_465]	1.36	0.84
1:A:130:SER:O	1:A:423:ARG:NH1[1_465]	1.38	0.82
1:B:131:GLY:CA	1:B:423:ARG:NH2[1_445]	1.39	0.81
1:B:131:GLY:C	1:B:423:ARG:NH1[1_445]	1.39	0.81
1:A:130:SER:C	1:A:423:ARG:NH1[1_465]	1.57	0.63
1:B:214:GLN:OE1	1:B:312:GLN:NE2[1_455]	1.61	0.59
1:B:131:GLY:O	1:B:423:ARG:NH1[1_445]	1.63	0.57
1:B:129:GLN:NE2	1:B:473:GLU:OE2[1_445]	1.65	0.55
1:B:131:GLY:N	1:B:423:ARG:CZ[1_445]	1.77	0.43
1:A:80:GLN:OE1	1:A:497:ARG:NH2[1_565]	1.95	0.25
1:A:131:GLY:CA	1:A:423:ARG:CZ[1_465]	1.98	0.22
2:A:742:HOH:O	2:B:739:HOH:O[1_655]	1.99	0.21
2:A:722:HOH:O	2:B:754:HOH:O[1_655]	2.01	0.19
1:B:130:SER:O	1:B:423:ARG:NH2[1_445]	2.03	0.17
1:A:130:SER:C	1:A:423:ARG:CZ[1_465]	2.13	0.07
1:A:131:GLY:N	1:A:423:ARG:CZ[1_465]	2.13	0.07
2:B:715:HOH:O	2:B:717:HOH:O[1_445]	2.13	0.07

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	437/447 (98%)	421 (96%)	14 (3%)	2 (0%)	24	31
1	B	436/447 (98%)	425 (98%)	8 (2%)	3 (1%)	18	23
All	All	873/894 (98%)	846 (97%)	22 (2%)	5 (1%)	21	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	HIS
1	B	248	LYS
1	A	300	ARG
1	A	249	PRO
1	B	252	ASP

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	376/381 (99%)	376 (100%)	0	100	100
1	B	375/381 (98%)	375 (100%)	0	100	100
All	All	751/762 (99%)	751 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	95	GLN
1	A	103	GLN
1	A	105	GLN
1	A	141	ASN
1	A	181	GLN
1	A	193	GLN
1	A	312	GLN
1	A	326	ASN
1	A	373	ASN
1	A	417	GLN
1	A	495	ASN
1	B	87	GLN
1	B	181	GLN
1	B	193	GLN
1	B	214	GLN
1	B	226	ASN

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Mol	Chain	Res	Type
1	B	294	GLN
1	B	334	HIS

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	439/447 (98%)	-1.38	0 100 100	18, 28, 48, 62	0
1	B	438/447 (97%)	-1.38	0 100 100	18, 28, 47, 69	0
All	All	877/894 (98%)	-1.38	0 100 100	18, 28, 47, 69	0

There are no RSRZ outliers to report.

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.