



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:56 AM EDT

PDB ID : 4XRK / pdb_00004xrk
Title : Crystal Structure of Importin Beta in a Polyethylene Glycol Condition
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Deposited on : 2015-01-21
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

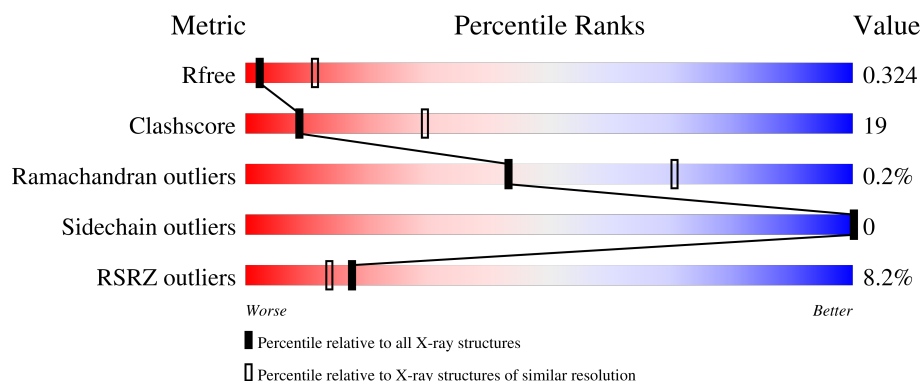
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	882	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6399 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 Beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6399	4001	1107	1251	40			

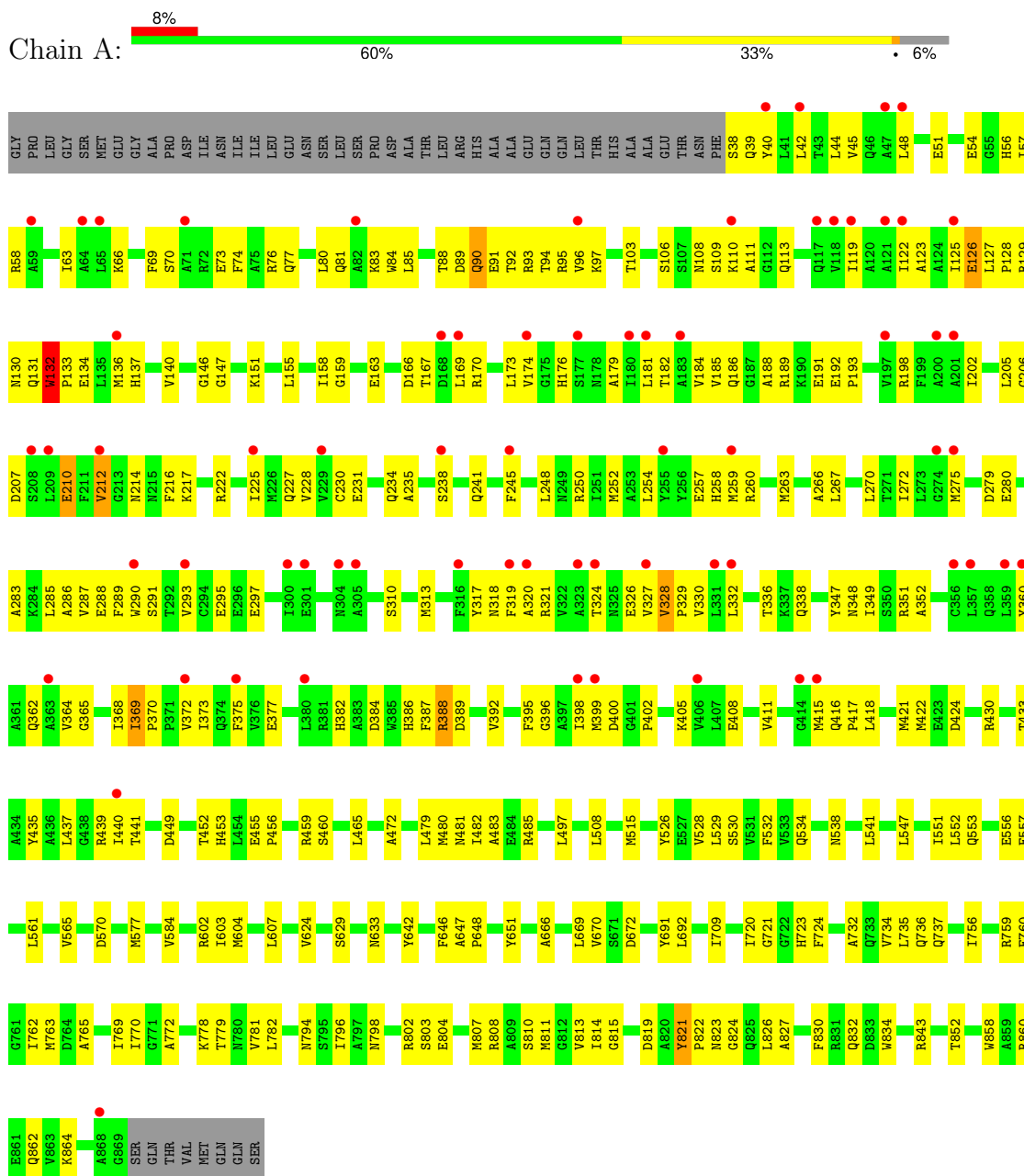
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP G0S143
A	-3	PRO	-	expression tag	UNP G0S143
A	-2	LEU	-	expression tag	UNP G0S143
A	-1	GLY	-	expression tag	UNP G0S143
A	0	SER	-	expression tag	UNP G0S143

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Importin Beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.41Å 121.19Å 132.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.64 – 3.25 44.64 – 3.25	Depositor EDS
% Data completeness (in resolution range)	95.1 (44.64-3.25) 95.0 (44.64-3.25)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.289 , 0.317 0.293 , 0.324	Depositor DCC
R_{free} test set	803 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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	0.41	1/6504 (0.0%)	0.87	12/8826 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	ARG	C-N	-6.34	1.25	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	GLN	N-CA-C	-10.86	99.75	113.43
1	A	126	GLU	N-CA-C	10.27	122.55	111.36
1	A	132	TRP	CA-C-N	-7.54	112.92	120.31
1	A	132	TRP	C-N-CA	-7.54	112.92	120.31
1	A	821	TYR	CA-C-N	6.57	126.51	119.28
1	A	821	TYR	C-N-CA	6.57	126.51	119.28
1	A	89	ASP	N-CA-C	5.90	123.37	110.80
1	A	328	VAL	CB-CA-C	-5.40	108.62	114.35
1	A	370	PRO	N-CA-C	5.37	117.25	110.70
1	A	212	VAL	N-CA-C	-5.34	107.27	112.29
1	A	210	GLU	N-CA-C	-5.16	105.78	111.71
1	A	369	ILE	CB-CA-C	-5.03	107.41	114.00

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	6399	0	6305	236	0
All	All	6399	0	6305	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (236) 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:227:GLN:O	1:A:231:GLU:HG2	1.63	0.99
1:A:123:ALA:HB1	1:A:127:LEU:HD23	1.54	0.90
1:A:332:LEU:HD22	1:A:375:PHE:HB3	1.60	0.84
1:A:123:ALA:O	1:A:127:LEU:HG	1.77	0.84
1:A:42:LEU:HD21	1:A:92:THR:HG21	1.64	0.80
1:A:808:ARG:HB2	1:A:852:THR:HG22	1.64	0.79
1:A:272:ILE:HD11	1:A:326:GLU:HB3	1.65	0.79
1:A:88:THR:CG2	1:A:91:GLU:HG2	2.15	0.76
1:A:263:MET:HA	1:A:267:LEU:HD12	1.69	0.75
1:A:91:GLU:HG3	1:A:92:THR:H	1.53	0.74
1:A:127:LEU:HD12	1:A:128:PRO:N	2.05	0.72
1:A:88:THR:HG22	1:A:91:GLU:CB	2.20	0.71
1:A:382:HIS:O	1:A:388:ARG:NH1	2.21	0.70
1:A:212:VAL:HG21	1:A:254:LEU:HD22	1.73	0.70
1:A:97:LYS:HG2	1:A:122:ILE:HD13	1.75	0.69
1:A:483:ALA:HA	1:A:497:LEU:HD11	1.73	0.69
1:A:92:THR:O	1:A:95:ARG:N	2.26	0.69
1:A:206:GLY:O	1:A:250:ARG:NH1	2.25	0.69
1:A:92:THR:HB	1:A:95:ARG:HB3	1.74	0.68
1:A:51:GLU:CD	1:A:58:ARG:HH12	2.01	0.68
1:A:127:LEU:HA	1:A:131:GLN:O	1.93	0.67
1:A:607:LEU:HD22	1:A:624:VAL:HG13	1.78	0.66
1:A:435:TYR:OH	1:A:439:ARG:NH2	2.28	0.66
1:A:88:THR:CG2	1:A:91:GLU:CB	2.74	0.65
1:A:155:LEU:HD23	1:A:158:ILE:HD12	1.79	0.65
1:A:123:ALA:HB1	1:A:127:LEU:CD2	2.27	0.64
1:A:384:ASP:HB3	1:A:387:PHE:HD2	1.62	0.63
1:A:248:LEU:HD22	1:A:289:PHE:HE1	1.62	0.63
1:A:92:THR:O	1:A:93:ARG:C	2.43	0.62
1:A:832:GLN:OE1	1:A:834:TRP:NE1	2.33	0.62
1:A:125:ILE:O	1:A:129:ARG:NH1	2.30	0.62
1:A:552:LEU:HD21	1:A:603:ILE:HG12	1.81	0.61
1:A:88:THR:CG2	1:A:91:GLU:CG	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:OD1	1:A:349:ILE:N	2.34	0.61
1:A:63:ILE:HG23	1:A:66:LYS:HE2	1.81	0.61
1:A:508:LEU:HD23	1:A:529:LEU:HB2	1.81	0.61
1:A:90:GLN:O	1:A:91:GLU:C	2.44	0.61
1:A:69:PHE:HA	1:A:80:LEU:HB3	1.84	0.60
1:A:166:ASP:HB3	1:A:169:LEU:HB3	1.84	0.59
1:A:84:TRP:HD1	1:A:85:LEU:HD12	1.66	0.59
1:A:170:ARG:HA	1:A:173:LEU:HB2	1.83	0.59
1:A:819:ASP:OD1	1:A:862:GLN:NE2	2.35	0.59
1:A:396:GLY:O	1:A:439:ARG:NE	2.35	0.59
1:A:91:GLU:HG3	1:A:92:THR:N	2.18	0.59
1:A:338:GLN:NE2	1:A:389:ASP:OD2	2.26	0.59
1:A:297:GLU:OE2	1:A:319:PHE:HB2	2.02	0.58
1:A:217:LYS:O	1:A:258:HIS:NE2	2.37	0.58
1:A:88:THR:CG2	1:A:91:GLU:HB2	2.33	0.58
1:A:140:VAL:HG21	1:A:179:ALA:HB1	1.85	0.57
1:A:320:ALA:O	1:A:324:THR:HG23	2.04	0.57
1:A:449:ASP:OD2	1:A:452:THR:HG22	2.03	0.57
1:A:763:MET:HE2	1:A:810:SER:HA	1.85	0.57
1:A:250:ARG:O	1:A:254:LEU:HG	2.05	0.57
1:A:422:MET:HG3	1:A:460:SER:OG	2.05	0.57
1:A:216:PHE:O	1:A:222:ARG:NE	2.38	0.57
1:A:88:THR:HG22	1:A:91:GLU:HB2	1.87	0.56
1:A:84:TRP:CZ2	1:A:93:ARG:HD2	2.41	0.56
1:A:373:ILE:O	1:A:377:GLU:HG3	2.06	0.56
1:A:88:THR:HG21	1:A:91:GLU:HG2	1.87	0.56
1:A:724:PHE:CE2	1:A:769:ILE:HG12	2.41	0.55
1:A:159:GLY:O	1:A:163:GLU:HG3	2.07	0.55
1:A:411:VAL:O	1:A:415:MET:HB2	2.06	0.55
1:A:80:LEU:HD23	1:A:83:LYS:HD3	1.88	0.55
1:A:267:LEU:HD23	1:A:270:LEU:HD12	1.87	0.55
1:A:804:GLU:HG2	1:A:852:THR:HG21	1.87	0.55
1:A:84:TRP:CE2	1:A:93:ARG:HD2	2.41	0.55
1:A:480:MET:HG3	1:A:528:VAL:HG22	1.88	0.55
1:A:97:LYS:HD3	1:A:126:GLU:OE1	2.07	0.55
1:A:395:PHE:HE2	1:A:440:ILE:HD11	1.70	0.55
1:A:779:THR:O	1:A:821:TYR:OH	2.24	0.54
1:A:119:ILE:HD12	1:A:132:TRP:HH2	1.72	0.54
1:A:289:PHE:O	1:A:293:VAL:HG23	2.07	0.54
1:A:692:LEU:HB3	1:A:709:ILE:HG23	1.88	0.54
1:A:347:TYR:HA	1:A:351:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:GLY:HA3	1:A:858:TRP:CZ3	2.42	0.54
1:A:126:GLU:O	1:A:131:GLN:HB2	2.06	0.54
1:A:320:ALA:HB1	1:A:364:VAL:HG22	1.89	0.54
1:A:235:ALA:O	1:A:241:GLN:NE2	2.41	0.53
1:A:92:THR:O	1:A:94:THR:N	2.41	0.53
1:A:424:ASP:O	1:A:430:ARG:NE	2.32	0.53
1:A:259:MET:O	1:A:263:MET:HG2	2.09	0.53
1:A:860:ARG:HG3	1:A:864:LYS:NZ	2.24	0.53
1:A:54:GLU:OE1	1:A:56:HIS:NE2	2.42	0.53
1:A:280:GLU:HA	1:A:349:ILE:HD11	1.91	0.53
1:A:92:THR:C	1:A:94:THR:N	2.67	0.52
1:A:170:ARG:O	1:A:174:VAL:HG23	2.08	0.52
1:A:770:ILE:HG12	1:A:782:LEU:HD21	1.91	0.52
1:A:182:THR:O	1:A:186:GLN:HG2	2.10	0.52
1:A:483:ALA:HB2	1:A:532:PHE:CD1	2.45	0.52
1:A:248:LEU:HD22	1:A:289:PHE:CE1	2.44	0.52
1:A:77:GLN:O	1:A:81:GLN:HG3	2.10	0.51
1:A:92:THR:OG1	1:A:96:VAL:HG23	2.10	0.51
1:A:275:MET:HB3	1:A:330:VAL:HG11	1.91	0.51
1:A:395:PHE:HZ	1:A:411:VAL:HG22	1.75	0.51
1:A:821:TYR:HD2	1:A:826:LEU:HD11	1.74	0.51
1:A:285:LEU:HD23	1:A:288:GLU:OE1	2.10	0.51
1:A:422:MET:SD	1:A:433:THR:CG2	2.98	0.51
1:A:127:LEU:HD12	1:A:128:PRO:CD	2.40	0.51
1:A:189:ARG:HB3	1:A:191:GLU:OE1	2.10	0.50
1:A:452:THR:HG23	1:A:453:HIS:ND1	2.26	0.50
1:A:128:PRO:C	1:A:130:ASN:H	2.20	0.50
1:A:147:GLY:O	1:A:151:LYS:HG3	2.11	0.50
1:A:481:ASN:O	1:A:485:ARG:HG2	2.12	0.50
1:A:804:GLU:CG	1:A:852:THR:HG21	2.42	0.50
1:A:756:ILE:O	1:A:760:GLU:HG3	2.12	0.50
1:A:465:LEU:HD12	1:A:472:ALA:HB1	1.94	0.49
1:A:565:VAL:HG13	1:A:570:ASP:HB2	1.95	0.49
1:A:106:SER:OG	1:A:111:ALA:HB3	2.12	0.49
1:A:84:TRP:CD1	1:A:85:LEU:HD12	2.46	0.49
1:A:317:TYR:HB3	1:A:319:PHE:CE1	2.48	0.49
1:A:287:VAL:HG11	1:A:352:ALA:HB1	1.95	0.49
1:A:530:SER:O	1:A:534:GLN:HG3	2.12	0.49
1:A:778:LYS:O	1:A:781:VAL:HG12	2.12	0.49
1:A:51:GLU:HA	1:A:58:ARG:NH1	2.28	0.49
1:A:651:TYR:HB3	1:A:691:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:ARG:NH1	1:A:860:ARG:HD3	2.27	0.49
1:A:285:LEU:CD2	1:A:288:GLU:OE1	2.61	0.48
1:A:88:THR:HG22	1:A:91:GLU:HB3	1.93	0.48
1:A:384:ASP:OD2	1:A:386:HIS:HB2	2.13	0.48
1:A:136:MET:HG2	1:A:176:HIS:CD2	2.49	0.48
1:A:384:ASP:HB3	1:A:387:PHE:CD2	2.46	0.48
1:A:163:GLU:HA	1:A:207:ASP:HB2	1.94	0.48
1:A:760:GLU:OE2	1:A:803:SER:OG	2.26	0.48
1:A:125:ILE:HG23	1:A:129:ARG:NH1	2.29	0.47
1:A:248:LEU:O	1:A:252:MET:HG3	2.13	0.47
1:A:245:PHE:HD1	1:A:289:PHE:CZ	2.32	0.47
1:A:372:VAL:HG11	1:A:398:ILE:HG21	1.97	0.47
1:A:369:ILE:HD11	1:A:402:PRO:HB3	1.96	0.47
1:A:418:LEU:CD1	1:A:433:THR:HG23	2.45	0.47
1:A:796:ILE:O	1:A:802:ARG:HD3	2.15	0.47
1:A:127:LEU:CD1	1:A:128:PRO:HD3	2.45	0.47
1:A:252:MET:SD	1:A:289:PHE:HD1	2.38	0.47
1:A:275:MET:CB	1:A:330:VAL:HG11	2.45	0.47
1:A:553:GLN:O	1:A:557:GLU:HG3	2.14	0.47
1:A:433:THR:O	1:A:437:LEU:HG	2.14	0.47
1:A:132:TRP:CG	1:A:132:TRP:O	2.67	0.47
1:A:515:MET:HE1	1:A:577:MET:HE1	1.97	0.46
1:A:629:SER:OG	1:A:672:ASP:OD2	2.24	0.46
1:A:132:TRP:O	1:A:132:TRP:CD1	2.68	0.46
1:A:84:TRP:CH2	1:A:122:ILE:HG12	2.50	0.46
1:A:186:GLN:OE1	1:A:189:ARG:NH2	2.49	0.46
1:A:735:LEU:HD21	1:A:765:ALA:HB3	1.97	0.46
1:A:74:PHE:O	1:A:77:GLN:HB3	2.16	0.46
1:A:666:ALA:O	1:A:670:VAL:HG23	2.15	0.46
1:A:260:ARG:HB3	1:A:317:TYR:CE1	2.51	0.46
1:A:88:THR:HG23	1:A:91:GLU:CG	2.44	0.46
1:A:252:MET:HA	1:A:259:MET:HE1	1.97	0.46
1:A:416:GLN:HB3	1:A:417:PRO:HD3	1.98	0.46
1:A:422:MET:SD	1:A:433:THR:HG22	2.55	0.46
1:A:88:THR:HB	1:A:93:ARG:NH1	2.31	0.46
1:A:455:GLU:HB3	1:A:456:PRO:HD3	1.98	0.46
1:A:257:GLU:HA	1:A:317:TYR:OH	2.17	0.45
1:A:647:ALA:HB3	1:A:648:PRO:HD3	1.99	0.45
1:A:181:LEU:O	1:A:185:VAL:HG23	2.17	0.45
1:A:629:SER:O	1:A:633:ASN:ND2	2.47	0.45
1:A:821:TYR:HA	1:A:822:PRO:HD2	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLU:HA	1:A:137:HIS:ND1	2.32	0.45
1:A:388:ARG:O	1:A:392:VAL:HG22	2.16	0.45
1:A:51:GLU:CD	1:A:58:ARG:NH1	2.73	0.45
1:A:291:SER:O	1:A:295:GLU:HG3	2.17	0.45
1:A:405:LYS:HA	1:A:408:GLU:HG2	1.97	0.45
1:A:538:ASN:HA	1:A:541:LEU:HG	1.99	0.45
1:A:807:MET:O	1:A:811:MET:HG2	2.17	0.45
1:A:275:MET:HE1	1:A:287:VAL:HG22	1.98	0.45
1:A:399:MET:HE1	1:A:411:VAL:HG21	1.99	0.44
1:A:108:ASN:ND2	1:A:110:LYS:HB2	2.32	0.44
1:A:362:GLN:HG2	1:A:400:ASP:OD2	2.18	0.44
1:A:482:ILE:HG22	1:A:497:LEU:HD21	1.99	0.44
1:A:167:THR:HA	1:A:170:ARG:HG2	1.99	0.44
1:A:73:GLU:OE1	1:A:76:ARG:N	2.40	0.44
1:A:169:LEU:O	1:A:173:LEU:HG	2.18	0.44
1:A:260:ARG:NE	1:A:317:TYR:HE1	2.16	0.44
1:A:860:ARG:HG3	1:A:864:LYS:HZ2	1.82	0.44
1:A:241:GLN:HB3	1:A:245:PHE:CE2	2.53	0.44
1:A:810:SER:O	1:A:814:ILE:HG13	2.17	0.44
1:A:40:TYR:CE2	1:A:44:LEU:HD11	2.53	0.43
1:A:202:ILE:HA	1:A:205:LEU:HD12	1.99	0.43
1:A:479:LEU:HD23	1:A:482:ILE:HD12	1.98	0.43
1:A:556:GLU:CD	1:A:602:ARG:HH11	2.26	0.43
1:A:557:GLU:O	1:A:561:LEU:HD13	2.18	0.43
1:A:823:ASN:OD1	1:A:824:GLY:N	2.51	0.43
1:A:123:ALA:CB	1:A:127:LEU:HD23	2.36	0.43
1:A:127:LEU:HD12	1:A:128:PRO:HD3	1.99	0.43
1:A:136:MET:HG2	1:A:176:HIS:HD2	1.83	0.43
1:A:365:GLY:O	1:A:368:ILE:HG22	2.19	0.43
1:A:310:SER:HA	1:A:313:MET:HG3	2.01	0.43
1:A:336:THR:O	1:A:386:HIS:HB3	2.19	0.43
1:A:455:GLU:OE2	1:A:459:ARG:NH2	2.51	0.43
1:A:38:SER:OG	1:A:39:GLN:N	2.52	0.43
1:A:45:VAL:O	1:A:48:LEU:HB3	2.18	0.43
1:A:732:ALA:O	1:A:736:GLN:HG3	2.19	0.43
1:A:418:LEU:HD11	1:A:433:THR:HG23	2.00	0.43
1:A:547:LEU:O	1:A:551:ILE:HG12	2.19	0.43
1:A:794:ASN:OD1	1:A:798:ASN:ND2	2.52	0.43
1:A:225:ILE:O	1:A:228:VAL:HG12	2.19	0.43
1:A:328:VAL:N	1:A:329:PRO:HD2	2.34	0.43
1:A:483:ALA:HB2	1:A:532:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PRO:HB3	1:A:375:PHE:CZ	2.54	0.42
1:A:646:PHE:HZ	1:A:669:LEU:HD21	1.84	0.42
1:A:259:MET:HG2	1:A:263:MET:HG2	2.00	0.42
1:A:48:LEU:HG	1:A:103:THR:HG21	2.01	0.42
1:A:827:ALA:HA	1:A:830:PHE:HB2	1.99	0.42
1:A:56:HIS:CE1	1:A:57:ILE:HG12	2.54	0.42
1:A:230:CYS:O	1:A:234:GLN:HG3	2.18	0.42
1:A:283:ALA:O	1:A:287:VAL:HG23	2.20	0.42
1:A:480:MET:HG2	1:A:528:VAL:HA	2.01	0.42
1:A:238:SER:HB2	1:A:279:ASP:OD2	2.20	0.42
1:A:131:GLN:C	1:A:133:PRO:HD3	2.45	0.42
1:A:97:LYS:HD2	1:A:132:TRP:CE3	2.55	0.41
1:A:181:LEU:HD12	1:A:216:PHE:CE2	2.55	0.41
1:A:66:LYS:O	1:A:70:SER:N	2.53	0.41
1:A:241:GLN:HB3	1:A:245:PHE:HE2	1.85	0.41
1:A:188:ALA:HA	1:A:198:ARG:HG2	2.02	0.41
1:A:88:THR:HG23	1:A:91:GLU:HG2	1.98	0.41
1:A:181:LEU:HA	1:A:184:VAL:HG22	2.01	0.41
1:A:192:GLU:CD	1:A:193:PRO:HD2	2.46	0.41
1:A:417:PRO:O	1:A:421:MET:HG3	2.21	0.41
1:A:133:PRO:O	1:A:134:GLU:HB2	2.21	0.41
1:A:109:SER:O	1:A:113:GLN:N	2.54	0.41
1:A:266:ALA:O	1:A:270:LEU:HG	2.20	0.41
1:A:483:ALA:HB2	1:A:532:PHE:HD1	1.86	0.41
1:A:526:TYR:HD1	1:A:584:VAL:HG21	1.85	0.41
1:A:556:GLU:OE2	1:A:602:ARG:NE	2.34	0.41
1:A:207:ASP:HA	1:A:210:GLU:HG3	2.03	0.41
1:A:604:MET:HG3	1:A:642:TYR:CG	2.56	0.41
1:A:734:VAL:O	1:A:737:GLN:HB3	2.20	0.41
1:A:286:ALA:HA	1:A:289:PHE:CD2	2.55	0.41
1:A:318:ASN:OD1	1:A:321:ARG:HB2	2.21	0.40
1:A:327:VAL:HG11	1:A:360:TYR:OH	2.22	0.40
1:A:759:ARG:HG2	1:A:762:ILE:HD12	2.02	0.40
1:A:721:GLY:O	1:A:772:ALA:HB1	2.21	0.40
1:A:290:TRP:HA	1:A:293:VAL:HB	2.04	0.40
1:A:441:THR:HG22	1:A:481:ASN:HB3	2.04	0.40
1:A:763:MET:HE3	1:A:813:VAL:HG21	2.03	0.40
1:A:146:GLY:O	1:A:151:LYS:HE3	2.22	0.40
1:A:720:ILE:CG2	1:A:723:HIS:HB2	2.52	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	830/882 (94%)	796 (96%)	32 (4%)	2 (0%)	43 70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	TRP
1	A	214	ASN

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	680/721 (94%)	680 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	451	ASN
1	A	503	GLN
1	A	657	GLN
1	A	704	GLN
1	A	723	HIS
1	A	798	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	832/882 (94%)	0.67	68 (8%) 17 14	42, 122, 216, 229	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	5.2
1	A	323	ALA	5.0
1	A	225	ILE	4.6
1	A	398	ILE	3.7
1	A	118	VAL	3.6
1	A	229	VAL	3.6
1	A	380	LEU	3.6
1	A	320	ALA	3.6
1	A	290	TRP	3.5
1	A	212	VAL	3.4
1	A	209	LEU	3.3
1	A	363	ALA	3.3
1	A	316	PHE	3.1
1	A	122	ILE	3.1
1	A	136	MET	3.0
1	A	415	MET	3.0
1	A	275	MET	3.0
1	A	201	ALA	2.9
1	A	255	TYR	2.9
1	A	208	SER	2.8
1	A	183	ALA	2.8
1	A	168	ASP	2.8
1	A	180	ILE	2.8
1	A	406	VAL	2.8
1	A	200	ALA	2.7
1	A	372	VAL	2.7
1	A	119	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	96	VAL	2.7
1	A	327	VAL	2.7
1	A	40	TYR	2.7
1	A	59	ALA	2.6
1	A	169	LEU	2.6
1	A	359	LEU	2.6
1	A	375	PHE	2.6
1	A	356	CYS	2.6
1	A	274	GLY	2.6
1	A	238	SER	2.5
1	A	197	VAL	2.5
1	A	259	MET	2.5
1	A	360	TYR	2.5
1	A	331	LEU	2.4
1	A	64	ALA	2.4
1	A	324	THR	2.4
1	A	301	GLU	2.4
1	A	125	ILE	2.3
1	A	332	LEU	2.3
1	A	177	SER	2.2
1	A	305	ALA	2.2
1	A	319	PHE	2.2
1	A	440	ILE	2.2
1	A	48	LEU	2.2
1	A	47	ALA	2.2
1	A	868	ALA	2.2
1	A	82	ALA	2.1
1	A	293	VAL	2.1
1	A	42	LEU	2.1
1	A	65	LEU	2.1
1	A	181	LEU	2.1
1	A	399	MET	2.1
1	A	357	LEU	2.1
1	A	71	ALA	2.1
1	A	304	ASN	2.0
1	A	245	PHE	2.0
1	A	414	GLY	2.0
1	A	110	LYS	2.0
1	A	117	GLN	2.0
1	A	174	VAL	2.0
1	A	300	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.