



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:07 am BST

PDB ID : 4XRK
Title : Crystal Structure of Importin Beta in a Polyethylene Glycol Condition
Authors : Tauchert, M.J.; Neumann, P.; Ficner, R.; Dickmanns, A.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

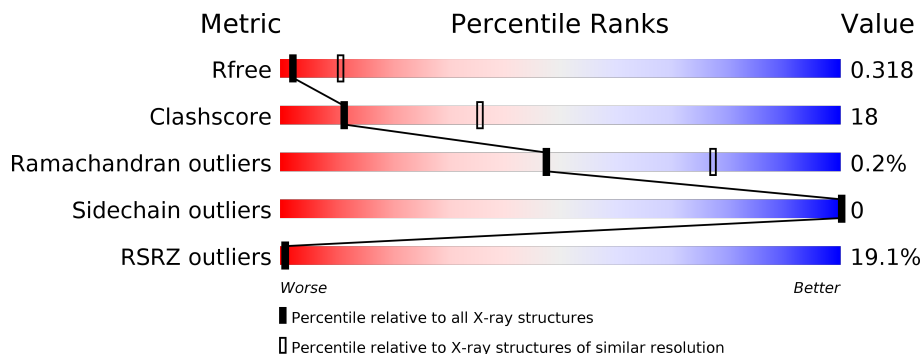
1 Overall quality at a glance

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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 on 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
			Total	C	N	O	S			
1	A	832	6399	4001	1107	1251	40	0	0	0

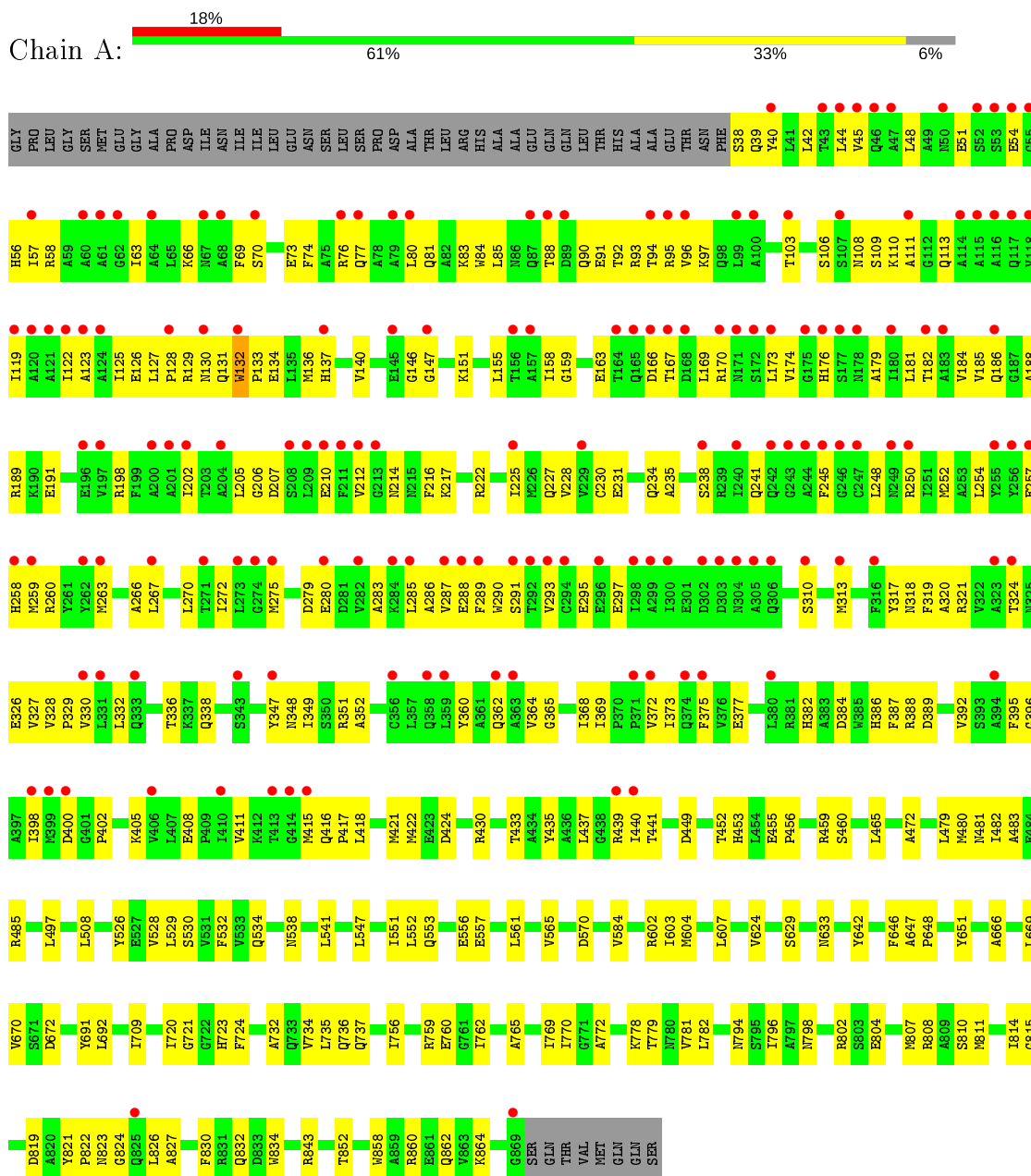
There are 5 discrepancies between the modelled and reference sequences:

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 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.

- 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) 95.1 (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)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.289 , 0.317 0.292 , 0.318	Depositor DCC
R_{free} test set	803 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtrriage
Anisotropy	0.350	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/6504	0.51	0/8826

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6399	0	6305	225	0
All	All	6399	0	6305	225	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 18.

All (225) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:51:GLU:CD	1:A:58:ARG:HH12	2.01	0.63
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: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
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: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:170:ARG:HA	1:A:173:LEU:HB2	1.83	0.59
1:A:84:TRP:HD1	1:A:85:LEU:HD12	1.66	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:338:GLN:NE2	1:A:389:ASP:OD2	2.26	0.59
1:A:91:GLU:HG3	1:A:92:THR:N	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:THR:O	1:A:93:ARG:C	2.43	0.57
1:A:449:ASP:OD2	1:A:452:THR:HG22	2.03	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:90:GLN:O	1:A:91:GLU:C	2.44	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:267:LEU:HD23	1:A:270:LEU:HD12	1.87	0.55
1:A:80:LEU:HD23	1:A:83:LYS:HD3	1.88	0.55
1:A:804:GLU:HG2	1:A:852:THR:HG21	1.87	0.55
1:A:480:MET:HG3	1:A:528:VAL:HG22	1.88	0.55
1:A:84:TRP:CE2	1:A:93:ARG:HD2	2.41	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
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:424:ASP:O	1:A:430:ARG:NE	2.32	0.53
1:A:92:THR:O	1:A:94:THR:N	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD22	1:A:289:PHE:CE1	2.44	0.52
1:A:275:MET:HB3	1:A:330:VAL:HG11	1.91	0.51
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: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: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:317:TYR:HB3	1:A:319:PHE:CE1	2.48	0.49
1:A:84:TRP:CD1	1:A:85:LEU:HD12	2.46	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
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:384:ASP:OD2	1:A:386:HIS:HB2	2.13	0.48
1:A:88:THR:HG22	1:A:91:GLU:HB3	1.93	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:92:THR:C	1:A:94:THR:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:132:TRP:CG	2.67	0.47
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: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:84:TRP:CH2	1:A:122:ILE:HG12	2.50	0.46
1:A:666:ALA:O	1:A:670:VAL:HG23	2.15	0.46
1:A:74:PHE:O	1:A:77:GLN:HB3	2.16	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: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:455:GLU:HB3	1:A:456:PRO:HD3	1.98	0.46
1:A:88:THR:HB	1:A:93:ARG:NH1	2.31	0.46
1:A:128:PRO:C	1:A:130:ASN:H	2.20	0.45
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
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: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: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: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:73:GLU:OE1	1:A:76:ARG:N	2.40	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:202:ILE:HA	1:A:205:LEU:HD12	1.99	0.43
1:A:40:TYR:CE2	1:A:44:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD23	1:A:482:ILE:HD12	1.98	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
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:181:LEU:HD12	1:A:216:PHE:CE2	2.55	0.41
1:A:97:LYS:HD2	1:A:132:TRP:CE3	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:181:LEU:HA	1:A:184:VAL:HG22	2.01	0.41
1:A:417:PRO:O	1:A:421:MET:HG3	2.21	0.41
1:A:88:THR:HG23	1:A:91:GLU:HG2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:734:VAL:O	1:A:737:GLN:HB3	2.20	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: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:51:GLU:CD	1:A:58:ARG:NH1	2.73	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 [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	830/882 (94%)	796 (96%)	32 (4%)	2 (0%)	47 77

All (2) Ramachandran outliers are listed below:

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

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	680/721 (94%)	680 (100%)	0	100 100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	A	241	GLN
1	A	657	GLN
1	A	704	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 carbohydrates 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

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%)	1.00	159 (19%) 1 1	42, 122, 216, 229	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	VAL	11.3
1	A	200	ALA	8.7
1	A	323	ALA	8.5
1	A	47	ALA	8.5
1	A	166	ASP	8.4
1	A	197	VAL	8.1
1	A	117	GLN	7.5
1	A	306	GLN	7.4
1	A	182	THR	7.0
1	A	121	ALA	6.7
1	A	44	LEU	6.5
1	A	210	GLU	6.2
1	A	242	GLN	6.1
1	A	316	PHE	6.0
1	A	170	ARG	6.0
1	A	183	ALA	5.9
1	A	80	LEU	5.8
1	A	302	ASP	5.7
1	A	171	ASN	5.6
1	A	165	GLN	5.6
1	A	122	ILE	5.4
1	A	99	LEU	5.3
1	A	167	THR	5.3
1	A	324	THR	5.3
1	A	398	ILE	5.3
1	A	259	MET	5.2
1	A	212	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	115	ALA	5.0
1	A	406	VAL	5.0
1	A	114	ALA	5.0
1	A	209	LEU	4.9
1	A	249	ASN	4.9
1	A	245	PHE	4.8
1	A	177	SER	4.7
1	A	292	THR	4.7
1	A	363	ALA	4.6
1	A	116	ALA	4.6
1	A	274	GLY	4.5
1	A	53	SER	4.5
1	A	100	ALA	4.5
1	A	103	THR	4.4
1	A	120	ALA	4.3
1	A	244	ALA	4.3
1	A	238	SER	4.3
1	A	64	ALA	4.2
1	A	208	SER	4.2
1	A	304	ASN	4.1
1	A	243	GLY	4.1
1	A	40	TYR	4.1
1	A	271	THR	4.1
1	A	77	GLN	4.1
1	A	305	ALA	4.0
1	A	96	VAL	4.0
1	A	415	MET	3.9
1	A	300	ILE	3.8
1	A	246	GLY	3.8
1	A	331	LEU	3.8
1	A	273	LEU	3.8
1	A	372	VAL	3.8
1	A	168	ASP	3.7
1	A	285	LEU	3.7
1	A	229	VAL	3.7
1	A	291	SER	3.7
1	A	256	TYR	3.7
1	A	60	ALA	3.7
1	A	119	ILE	3.6
1	A	333	GLN	3.6
1	A	211	PHE	3.6
1	A	128	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	61	ALA	3.6
1	A	201	ALA	3.5
1	A	280	GLU	3.5
1	A	213	GLY	3.5
1	A	123	ALA	3.5
1	A	70	SER	3.4
1	A	258	HIS	3.4
1	A	196	GLU	3.4
1	A	172	SER	3.4
1	A	313	MET	3.3
1	A	176	HIS	3.3
1	A	869	GLY	3.3
1	A	186	GLN	3.3
1	A	54	GLU	3.2
1	A	362	GLN	3.2
1	A	76	ARG	3.2
1	A	95	ARG	3.2
1	A	164	THR	3.1
1	A	414	GLY	3.1
1	A	52	SER	3.1
1	A	124	ALA	3.1
1	A	46	GLN	3.1
1	A	343	SER	3.1
1	A	347	TYR	3.1
1	A	45	VAL	3.1
1	A	137	HIS	3.1
1	A	89	ASP	3.0
1	A	247	CYS	2.9
1	A	79	ALA	2.8
1	A	263	MET	2.8
1	A	255	TYR	2.8
1	A	262	TYR	2.8
1	A	413	THR	2.8
1	A	825	GLN	2.8
1	A	371	PRO	2.8
1	A	111	ALA	2.8
1	A	257	GLU	2.8
1	A	178	ASN	2.7
1	A	250	ARG	2.7
1	A	225	ILE	2.7
1	A	375	PHE	2.6
1	A	132	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	310	SER	2.6
1	A	400	ASP	2.6
1	A	55	GLY	2.6
1	A	67	ASN	2.6
1	A	289	PHE	2.5
1	A	62	GLY	2.5
1	A	68	ALA	2.5
1	A	175	GLY	2.5
1	A	293	VAL	2.5
1	A	202	ILE	2.5
1	A	43	THR	2.5
1	A	380	LEU	2.4
1	A	145	GLU	2.4
1	A	330	VAL	2.4
1	A	374	GLN	2.4
1	A	284	LYS	2.4
1	A	147	GLY	2.4
1	A	294	CYS	2.4
1	A	240	ILE	2.4
1	A	296	GLU	2.4
1	A	57	ILE	2.4
1	A	157	ALA	2.3
1	A	410	ILE	2.3
1	A	440	ILE	2.3
1	A	50	ASN	2.2
1	A	356	CYS	2.2
1	A	359	LEU	2.2
1	A	282	VAL	2.2
1	A	130	ASN	2.2
1	A	298	ILE	2.2
1	A	439	ARG	2.2
1	A	275	MET	2.2
1	A	299	ALA	2.2
1	A	173	LEU	2.2
1	A	180	ILE	2.2
1	A	87	GLN	2.1
1	A	394	ALA	2.1
1	A	88	THR	2.1
1	A	94	THR	2.1
1	A	156	THR	2.1
1	A	107	SER	2.1
1	A	287	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLU	2.1
1	A	267	LEU	2.1
1	A	399	MET	2.1
1	A	303	ASP	2.1
1	A	358	GLN	2.0
1	A	204	ALA	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 carbohydrates 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.