Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:30 am BST

PDB ID	:	6FVB
Title	:	Structure of Lph2 , a novel bidirectional nuclear transport receptor in S. cerevisiae
Authors	:	Vera Rodriguez, A.; Huyton, T.; Gorlich, D.
Deposited on	:	2018-03-01
Resolution	:	3.30 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 ①) were used in the production of this report:

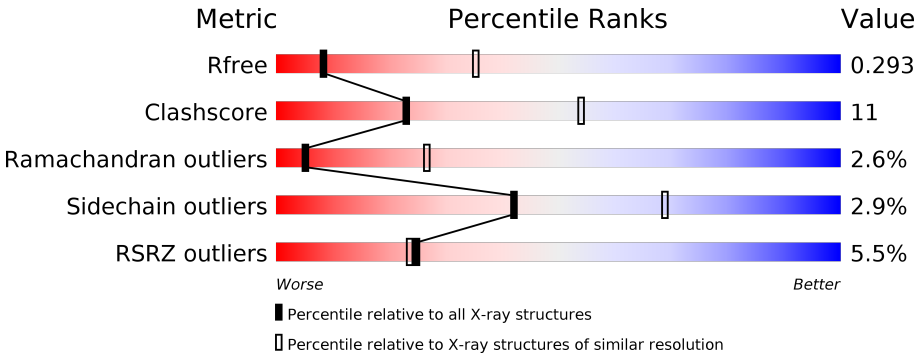
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	1031	5% 76% 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16442 atoms, of which 8253 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-like protein KAP120.

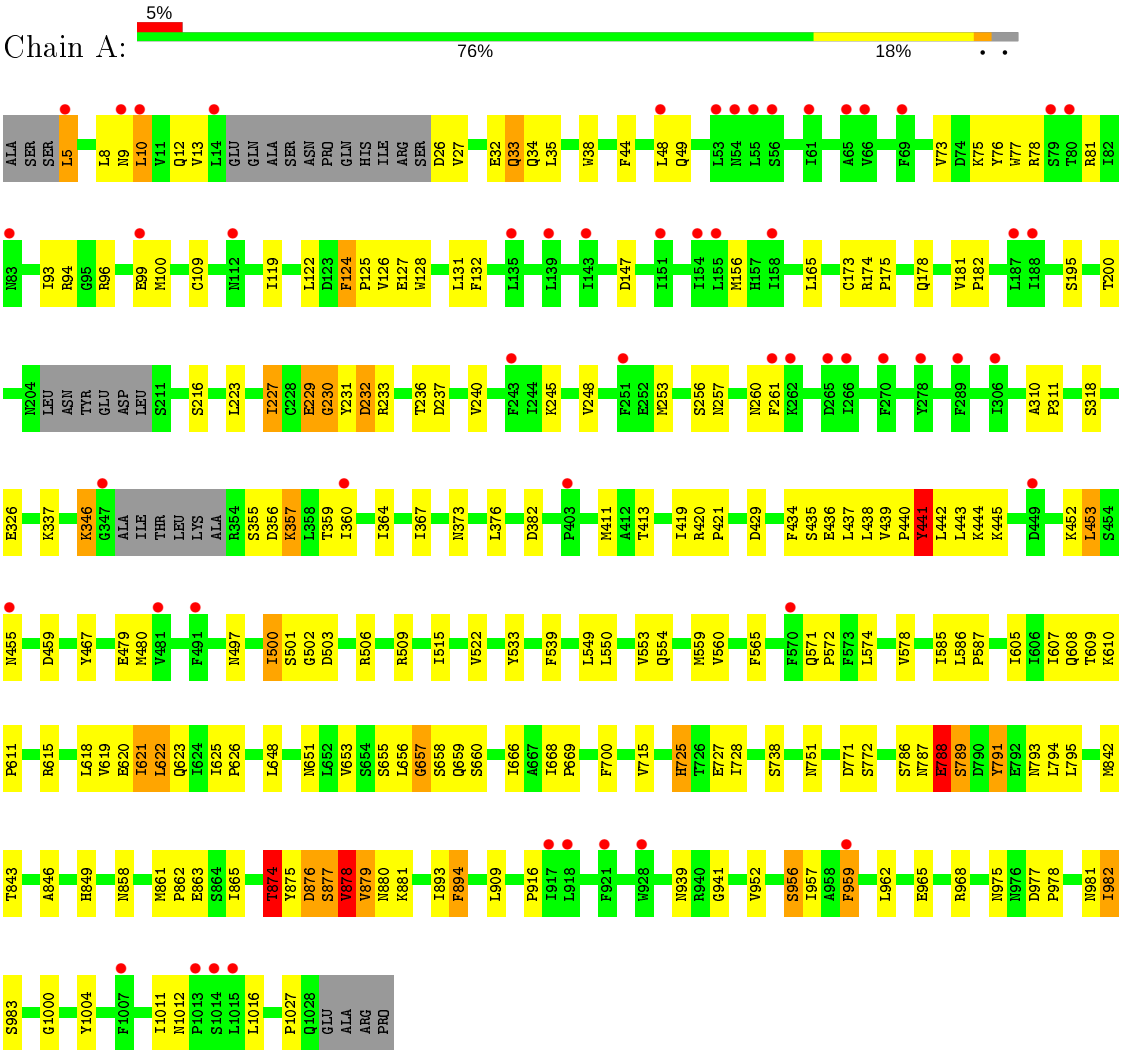
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	1001	16442	5274	8253	1351	1532	14	18	0	0	0

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-like protein KAP120

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.85Å 139.85Å 148.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.30 49.44 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.45-3.30) 99.9 (49.44-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.33Å)	Xtriage
Refinement program	PHENIX (dev_2873: ???)	Depositor
R, R_{free}	0.237 , 0.282 0.246 , 0.293	Depositor DCC
R_{free} test set	1137 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	144.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 95.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16442	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.34	0/8335	0.50	1/11281 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	441	TYR	C-N-CA	-5.21	108.68	121.70

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	8189	8253	8256	188	1
All	All	8189	8253	8256	188	1

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 11.

All (188) 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:441:TYR:CE1	1:A:445:LYS:HG3	1.82	1.14
1:A:382:ASP:OD1	1:A:441:TYR:HE2	1.28	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:SER:HB2	1:A:359:THR:OG1	1.50	1.11
1:A:441:TYR:HE1	1:A:445:LYS:HG3	1.10	1.10
1:A:878:VAL:O	1:A:916:PRO:CB	2.05	1.04
1:A:49:GLN:NE2	1:A:96:ARG:O	1.92	1.03
1:A:615:ARG:NH2	1:A:659:GLN:OE1	1.91	1.03
1:A:842:MSE:HE3	1:A:909:LEU:HD11	1.40	1.03
1:A:382:ASP:OD1	1:A:441:TYR:CE2	2.14	1.00
1:A:49:GLN:OE1	1:A:93:ILE:HG23	1.69	0.93
1:A:574:LEU:HD22	1:A:609:THR:HG21	1.49	0.92
1:A:651:ASN:O	1:A:655:SER:OG	1.88	0.90
1:A:878:VAL:O	1:A:916:PRO:HB2	1.70	0.89
1:A:441:TYR:CE1	1:A:445:LYS:CG	2.57	0.88
1:A:77:TRP:CE2	1:A:119:ILE:HG12	2.12	0.85
1:A:355:SER:HB3	1:A:359:THR:HB	1.58	0.84
1:A:355:SER:CB	1:A:359:THR:OG1	2.27	0.81
1:A:858:ASN:HA	1:A:861:MSE:HE2	1.61	0.81
1:A:77:TRP:CZ2	1:A:119:ILE:HG23	2.15	0.81
1:A:73:VAL:O	1:A:77:TRP:HB2	1.82	0.79
1:A:862:PRO:HD2	1:A:865:ILE:HD11	1.66	0.76
1:A:75:LYS:O	1:A:81:ARG:NH2	2.18	0.75
1:A:878:VAL:HB	1:A:916:PRO:HB3	1.68	0.74
1:A:878:VAL:HB	1:A:916:PRO:CG	2.16	0.74
1:A:441:TYR:CD1	1:A:445:LYS:CG	2.71	0.74
1:A:622:LEU:HD23	1:A:666:ILE:HG13	1.70	0.73
1:A:441:TYR:CD1	1:A:445:LYS:HG2	2.24	0.73
1:A:355:SER:CB	1:A:359:THR:CB	2.67	0.72
1:A:842:MSE:CE	1:A:909:LEU:HD11	2.19	0.72
1:A:657:GLY:O	1:A:659:GLN:N	2.22	0.72
1:A:435:SER:O	1:A:436:GLU:OE1	2.08	0.71
1:A:878:VAL:HB	1:A:916:PRO:HG3	1.73	0.70
1:A:787:ASN:HD22	1:A:795:LEU:HB2	1.56	0.70
1:A:437:LEU:CD1	1:A:480:MSE:HG3	2.22	0.69
1:A:437:LEU:HD23	1:A:437:LEU:N	2.06	0.69
1:A:5:LEU:N	1:A:5:LEU:HD23	2.06	0.69
1:A:878:VAL:HB	1:A:916:PRO:CB	2.24	0.68
1:A:77:TRP:HZ2	1:A:119:ILE:HG23	1.57	0.68
1:A:878:VAL:O	1:A:916:PRO:HB3	1.94	0.68
1:A:10:LEU:HD23	1:A:35:LEU:HD11	1.76	0.68
1:A:256:SER:O	1:A:260:ASN:ND2	2.26	0.67
1:A:77:TRP:CZ2	1:A:119:ILE:CG2	2.77	0.67
1:A:227:ILE:HD13	1:A:240:VAL:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TRP:CD1	1:A:122:LEU:HD12	2.29	0.67
1:A:77:TRP:CZ2	1:A:119:ILE:HG12	2.31	0.65
1:A:10:LEU:HD23	1:A:35:LEU:CD1	2.27	0.65
1:A:355:SER:HB2	1:A:359:THR:HG1	1.61	0.65
1:A:32:GLU:O	1:A:34:GLN:N	2.31	0.64
1:A:77:TRP:HD1	1:A:122:LEU:HD12	1.63	0.64
1:A:439:VAL:O	1:A:442:LEU:N	2.30	0.64
1:A:8:LEU:HD21	1:A:12:GLN:OE1	1.98	0.64
1:A:355:SER:CB	1:A:359:THR:HB	2.27	0.63
1:A:787:ASN:ND2	1:A:795:LEU:HB2	2.12	0.63
1:A:200:THR:HG23	1:A:253:MSE:HE1	1.78	0.63
1:A:574:LEU:CD2	1:A:609:THR:HG21	2.25	0.63
1:A:10:LEU:CD2	1:A:35:LEU:HD11	2.29	0.62
1:A:877:SER:O	1:A:880:ASN:HB2	1.99	0.62
1:A:502:GLY:O	1:A:506:ARG:HD3	2.00	0.61
1:A:232:ASP:OD1	1:A:232:ASP:N	2.32	0.61
1:A:337:LYS:NZ	1:A:429:ASP:OD2	2.31	0.60
1:A:436:GLU:OE1	1:A:436:GLU:HA	2.02	0.59
1:A:355:SER:HB3	1:A:359:THR:CB	2.27	0.59
1:A:99:GLU:HG3	1:A:100:MSE:HE2	1.84	0.59
1:A:607:ILE:HD11	1:A:651:ASN:ND2	2.18	0.59
1:A:360:ILE:HG22	1:A:360:ILE:O	2.02	0.58
1:A:435:SER:OG	1:A:435:SER:O	2.17	0.58
1:A:441:TYR:CD1	1:A:445:LYS:HG3	2.31	0.58
1:A:8:LEU:HD23	1:A:8:LEU:O	2.03	0.58
1:A:77:TRP:HZ2	1:A:119:ILE:CG2	2.16	0.58
1:A:77:TRP:HD1	1:A:122:LEU:CD1	2.16	0.58
1:A:849:HIS:NE2	1:A:874:THR:O	2.37	0.58
1:A:657:GLY:C	1:A:659:GLN:H	2.07	0.57
1:A:479:GLU:N	1:A:479:GLU:OE1	2.37	0.57
1:A:441:TYR:HD1	1:A:445:LYS:HG2	1.67	0.57
1:A:434:PHE:CD1	1:A:434:PHE:N	2.71	0.56
1:A:878:VAL:O	1:A:916:PRO:CG	2.53	0.56
1:A:441:TYR:HD1	1:A:441:TYR:O	1.88	0.56
1:A:842:MSE:HE3	1:A:909:LEU:CD1	2.26	0.56
1:A:609:THR:O	1:A:609:THR:HG22	2.05	0.56
1:A:618:LEU:HD22	1:A:656:LEU:HD21	1.89	0.55
1:A:727:GLU:OE1	1:A:727:GLU:N	2.33	0.55
1:A:622:LEU:CD2	1:A:666:ILE:HG13	2.34	0.55
1:A:509:ARG:HG3	1:A:539:PHE:CZ	2.41	0.55
1:A:479:GLU:O	1:A:480:MSE:HE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:O	1:A:38:TRP:HZ3	1.89	0.55
1:A:453:LEU:HD12	1:A:459:ASP:H	1.72	0.55
1:A:440:PRO:O	1:A:444:LYS:N	2.22	0.54
1:A:574:LEU:O	1:A:578:VAL:HG23	2.08	0.53
1:A:437:LEU:HD13	1:A:480:MSE:HG3	1.90	0.53
1:A:894:PHE:N	1:A:894:PHE:CD1	2.77	0.52
1:A:975:ASN:O	1:A:981:ASN:ND2	2.42	0.52
1:A:622:LEU:CD2	1:A:666:ILE:CG1	2.88	0.52
1:A:174:ARG:NH2	1:A:229:GLU:OE1	2.43	0.52
1:A:622:LEU:HD23	1:A:666:ILE:CG1	2.38	0.52
1:A:879:VAL:HG12	1:A:879:VAL:O	2.09	0.52
1:A:326:GLU:HG3	1:A:419:ILE:HB	1.91	0.51
1:A:382:ASP:CG	1:A:441:TYR:HE2	2.08	0.51
1:A:618:LEU:CD2	1:A:656:LEU:HD21	2.41	0.51
1:A:346:LYS:HB2	1:A:360:ILE:HG21	1.94	0.50
1:A:34:GLN:O	1:A:38:TRP:CZ3	2.64	0.50
1:A:607:ILE:HD11	1:A:651:ASN:CG	2.32	0.50
1:A:610:LYS:N	1:A:611:PRO:CD	2.75	0.49
1:A:941:GLY:HA3	1:A:983:SER:HA	1.94	0.49
1:A:738:SER:HA	1:A:965:GLU:OE2	2.13	0.49
1:A:571:GLN:N	1:A:572:PRO:CD	2.76	0.49
1:A:1011:ILE:O	1:A:1016:LEU:HD12	2.12	0.49
1:A:956:SER:OG	1:A:957:ILE:N	2.46	0.49
1:A:355:SER:HG	1:A:359:THR:H	1.55	0.48
1:A:356:ASP:O	1:A:357:LYS:HB2	2.13	0.48
1:A:440:PRO:HA	1:A:443:LEU:HB2	1.95	0.48
1:A:49:GLN:OE1	1:A:93:ILE:CG2	2.51	0.48
1:A:245:LYS:O	1:A:248:VAL:N	2.46	0.48
1:A:77:TRP:CE2	1:A:119:ILE:HG23	2.50	0.47
1:A:533:TYR:HH	1:A:565:PHE:HE1	1.62	0.47
1:A:880:ASN:O	1:A:881:LYS:C	2.53	0.47
1:A:126:VAL:O	1:A:127:GLU:HB2	2.14	0.47
1:A:174:ARG:HB3	1:A:175:PRO:HD3	1.96	0.47
1:A:245:LYS:O	1:A:248:VAL:HB	2.14	0.47
1:A:560:VAL:HG12	1:A:608:GLN:HG3	1.95	0.47
1:A:791:TYR:O	1:A:791:TYR:CG	2.67	0.47
1:A:310:ALA:HB3	1:A:311:PRO:HD3	1.96	0.47
1:A:668:ILE:HB	1:A:669:PRO:HD3	1.97	0.46
1:A:618:LEU:HD13	1:A:656:LEU:HD22	1.97	0.46
1:A:77:TRP:CZ2	1:A:119:ILE:CG1	2.99	0.46
1:A:373:ASN:OD1	1:A:376:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:TYR:CE1	1:A:559:MSE:HE2	2.50	0.46
1:A:94:ARG:HD3	1:A:128:TRP:CG	2.50	0.46
1:A:615:ARG:O	1:A:619:VAL:HG23	2.16	0.45
1:A:109:CYS:SG	1:A:156:MSE:SE	3.25	0.45
1:A:165:LEU:HD22	1:A:173:CYS:SG	2.57	0.45
1:A:725:HIS:HB3	1:A:728:ILE:HG12	1.98	0.45
1:A:941:GLY:HA3	1:A:982:ILE:O	2.17	0.45
1:A:420:ARG:HB3	1:A:421:PRO:HD3	1.99	0.44
1:A:894:PHE:N	1:A:894:PHE:HD1	2.15	0.44
1:A:437:LEU:HD11	1:A:480:MSE:HG3	1.98	0.44
1:A:715:VAL:HG11	1:A:751:ASN:OD1	2.18	0.44
1:A:791:TYR:HB2	1:A:794:LEU:HB3	1.99	0.44
1:A:874:THR:C	1:A:876:ASP:H	2.20	0.44
1:A:956:SER:O	1:A:959:PHE:N	2.41	0.44
1:A:411:MSE:HE2	1:A:550:LEU:HD13	1.99	0.44
1:A:233:ARG:O	1:A:236:THR:HG22	2.17	0.44
1:A:364:ILE:O	1:A:367:ILE:HG22	2.18	0.44
1:A:878:VAL:CB	1:A:916:PRO:HB3	2.43	0.44
1:A:467:TYR:HB3	1:A:515:ILE:HD11	1.99	0.44
1:A:49:GLN:OE1	1:A:93:ILE:HA	2.18	0.44
1:A:452:LYS:O	1:A:453:LEU:C	2.56	0.43
1:A:109:CYS:HB3	1:A:156:MSE:SE	2.68	0.43
1:A:1011:ILE:O	1:A:1012:ASN:C	2.57	0.43
1:A:439:VAL:N	1:A:440:PRO:CD	2.81	0.43
1:A:653:VAL:HG13	1:A:660:SER:HB2	2.00	0.43
1:A:894:PHE:HD1	1:A:894:PHE:H	1.67	0.43
1:A:625:ILE:HD11	1:A:648:LEU:HD23	2.01	0.43
1:A:787:ASN:O	1:A:788:GLU:C	2.58	0.43
1:A:181:VAL:N	1:A:182:PRO:CD	2.82	0.42
1:A:952:VAL:HG13	1:A:962:LEU:CD1	2.49	0.42
1:A:1000:GLY:O	1:A:1004:TYR:N	2.45	0.42
1:A:10:LEU:HD22	1:A:35:LEU:HD21	2.01	0.42
1:A:77:TRP:CD1	1:A:122:LEU:CD1	2.97	0.42
1:A:195:SER:CB	1:A:216:SER:HG	2.29	0.42
1:A:878:VAL:C	1:A:880:ASN:H	2.22	0.42
1:A:982:ILE:HD13	1:A:982:ILE:N	2.35	0.42
1:A:131:LEU:O	1:A:132:PHE:HB2	2.20	0.42
1:A:76:TYR:O	1:A:77:TRP:C	2.58	0.42
1:A:497:ASN:ND2	1:A:500:ILE:HD13	2.35	0.42
1:A:560:VAL:HG11	1:A:605:ILE:HA	2.01	0.42
1:A:700:PHE:O	1:A:968:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HG2	1:A:230:GLY:HA2	2.02	0.42
1:A:257:ASN:HA	1:A:260:ASN:HB2	2.03	0.41
1:A:789:SER:O	1:A:791:TYR:O	2.38	0.41
1:A:843:THR:O	1:A:846:ALA:HB3	2.20	0.41
1:A:621:ILE:O	1:A:625:ILE:HG12	2.21	0.41
1:A:13:VAL:HA	1:A:32:GLU:CB	2.51	0.41
1:A:49:GLN:OE1	1:A:93:ILE:HG12	2.21	0.41
1:A:549:LEU:O	1:A:553:VAL:HG23	2.20	0.41
1:A:620:GLU:O	1:A:623:GLN:HB3	2.20	0.41
1:A:223:LEU:O	1:A:227:ILE:HG13	2.21	0.41
1:A:656:LEU:O	1:A:657:GLY:O	2.39	0.41
1:A:878:VAL:O	1:A:880:ASN:N	2.54	0.41
1:A:622:LEU:O	1:A:626:PRO:HD3	2.21	0.41
1:A:33:GLN:HA	1:A:33:GLN:NE2	2.35	0.41
1:A:771:ASP:OD1	1:A:772:SER:N	2.54	0.40
1:A:786:SER:O	1:A:788:GLU:N	2.54	0.40
1:A:977:ASP:O	1:A:978:PRO:C	2.60	0.40
1:A:231:TYR:HE2	1:A:237:ASP:OD2	2.04	0.40
1:A:124:PHE:HB3	1:A:125:PRO:CD	2.51	0.40
1:A:586:LEU:HB3	1:A:587:PRO:HD3	2.03	0.40
1:A:874:THR:OG1	1:A:875:TYR:N	2.52	0.40
1:A:44:PHE:CE2	1:A:48:LEU:HD11	2.56	0.40

All (1) 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:A:81:ARG:HH11	1:A:620:GLU:HG2[8_665]	1.20	0.40

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	995/1031 (96%)	893 (90%)	76 (8%)	26 (3%)	5 27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	124	PHE
1	A	346	LYS
1	A	658	SER
1	A	357	LYS
1	A	453	LEU
1	A	657	GLY
1	A	788	GLU
1	A	793	ASN
1	A	874	THR
1	A	879	VAL
1	A	956	SER
1	A	413	THR
1	A	501	SER
1	A	725	HIS
1	A	789	SER
1	A	863	GLU
1	A	939	ASN
1	A	230	GLY
1	A	261	PHE
1	A	455	ASN
1	A	522	VAL
1	A	1027	PRO
1	A	147	ASP
1	A	878	VAL
1	A	585	ILE

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	934/942 (99%)	907 (97%)	27 (3%)	42 69

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	ASN
1	A	10	LEU
1	A	26	ASP
1	A	27	VAL
1	A	78	ARG
1	A	227	ILE
1	A	229	GLU
1	A	232	ASP
1	A	318	SER
1	A	438	LEU
1	A	441	TYR
1	A	500	ILE
1	A	503	ASP
1	A	554	GLN
1	A	621	ILE
1	A	622	LEU
1	A	788	GLU
1	A	791	TYR
1	A	874	THR
1	A	876	ASP
1	A	877	SER
1	A	878	VAL
1	A	893	ILE
1	A	894	PHE
1	A	959	PHE
1	A	982	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	983/1031 (95%)	0.38	54 (5%) 25 23	87, 146, 211, 262	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	LEU	6.4
1	A	154	ILE	6.3
1	A	449	ASP	5.9
1	A	65	ALA	5.7
1	A	347	GLY	5.4
1	A	262	LYS	5.2
1	A	69	PHE	5.1
1	A	83	ASN	4.4
1	A	54	ASN	4.2
1	A	270	PHE	4.1
1	A	455	ASN	3.9
1	A	403	PRO	3.9
1	A	921	PHE	3.8
1	A	251	PHE	3.8
1	A	9	ASN	3.6
1	A	491	PHE	3.6
1	A	928	TRP	3.6
1	A	918	LEU	3.5
1	A	1014	SER	3.5
1	A	155	LEU	3.4
1	A	158	ILE	3.3
1	A	187	LEU	3.2
1	A	56	SER	3.0
1	A	917	ILE	2.9
1	A	360	ILE	2.9
1	A	289	PHE	2.9
1	A	265	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	55	LEU	2.7
1	A	188	ILE	2.7
1	A	66	VAL	2.7
1	A	481	VAL	2.6
1	A	1015	LEU	2.6
1	A	14	LEU	2.6
1	A	261	PHE	2.6
1	A	5	LEU	2.6
1	A	151	ILE	2.6
1	A	278	TYR	2.5
1	A	53	LEU	2.5
1	A	139	LEU	2.5
1	A	80	THR	2.5
1	A	266	ILE	2.5
1	A	79	SER	2.3
1	A	112	ASN	2.3
1	A	1013	PRO	2.2
1	A	959	PHE	2.2
1	A	306	ILE	2.1
1	A	570	PHE	2.1
1	A	48	LEU	2.1
1	A	1007	PHE	2.1
1	A	61	ILE	2.1
1	A	143	ILE	2.1
1	A	99	GLU	2.0
1	A	243	PHE	2.0
1	A	135	LEU	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.