Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 12:02 PM EDT

PDB ID	:	7MW1
Title	:	Crystal structure of the Homo sapiens NUP93-NUP53 complex (NUP93 residues 174-819; NUP53 residues 84-150)
Authors	:	Petrovic, S.; Samanta, D.; Perriches, T.; Bley, C.J.; Thierbach, K.; Brown, B.; Nie, S.; Mobbs, G.W.; Stevens, T.A.; Liu, X.; Tomaleri, G.P.; Schaus, L.; Hoelz, A.
Deposited on	:	2021-05-15
Resolution	:	3.40 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:

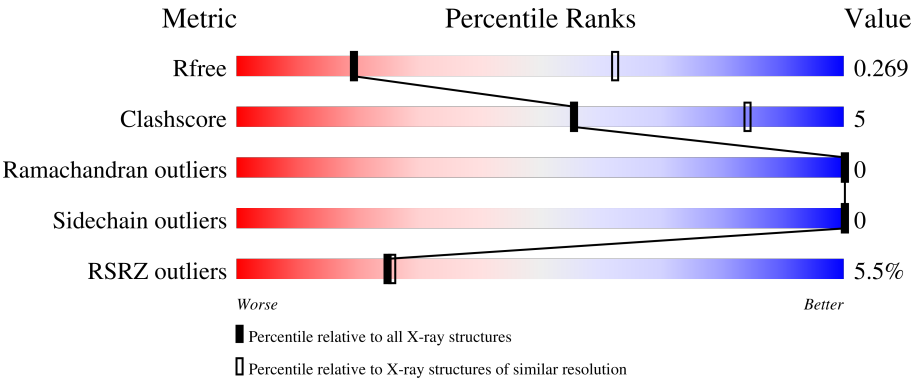
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	672	6% 81% 12% 8%
1	B	672	4% 81% 11% 8%
2	C	68	9% . 88%
2	D	68	9% . 88%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20384 atoms, of which 10190 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 Nuclear pore complex protein Nup93.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	621	Total	C	H	N	O	S	0	0	0
			10064	3200	5030	874	934	26			
1	B	621	Total	C	H	N	O	S	0	0	0
			10064	3200	5030	874	934	26			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	SER	-	expression tag	UNP Q8N1F7
A	149	SER	-	expression tag	UNP Q8N1F7
A	150	GLY	-	expression tag	UNP Q8N1F7
A	151	LEU	-	expression tag	UNP Q8N1F7
A	152	ASN	-	expression tag	UNP Q8N1F7
A	153	ASP	-	expression tag	UNP Q8N1F7
A	154	ILE	-	expression tag	UNP Q8N1F7
A	155	PHE	-	expression tag	UNP Q8N1F7
A	156	GLU	-	expression tag	UNP Q8N1F7
A	157	ALA	-	expression tag	UNP Q8N1F7
A	158	GLN	-	expression tag	UNP Q8N1F7
A	159	LYS	-	expression tag	UNP Q8N1F7
A	160	ILE	-	expression tag	UNP Q8N1F7
A	161	GLU	-	expression tag	UNP Q8N1F7
A	162	TRP	-	expression tag	UNP Q8N1F7
A	163	HIS	-	expression tag	UNP Q8N1F7
A	164	GLU	-	expression tag	UNP Q8N1F7
A	165	GLY	-	expression tag	UNP Q8N1F7
A	166	SER	-	expression tag	UNP Q8N1F7
A	167	ALA	-	expression tag	UNP Q8N1F7
A	168	GLY	-	expression tag	UNP Q8N1F7
A	169	GLY	-	expression tag	UNP Q8N1F7
A	170	SER	-	expression tag	UNP Q8N1F7
A	171	GLY	-	expression tag	UNP Q8N1F7
A	172	GLY	-	expression tag	UNP Q8N1F7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	SER	-	expression tag	UNP Q8N1F7
B	148	SER	-	expression tag	UNP Q8N1F7
B	149	SER	-	expression tag	UNP Q8N1F7
B	150	GLY	-	expression tag	UNP Q8N1F7
B	151	LEU	-	expression tag	UNP Q8N1F7
B	152	ASN	-	expression tag	UNP Q8N1F7
B	153	ASP	-	expression tag	UNP Q8N1F7
B	154	ILE	-	expression tag	UNP Q8N1F7
B	155	PHE	-	expression tag	UNP Q8N1F7
B	156	GLU	-	expression tag	UNP Q8N1F7
B	157	ALA	-	expression tag	UNP Q8N1F7
B	158	GLN	-	expression tag	UNP Q8N1F7
B	159	LYS	-	expression tag	UNP Q8N1F7
B	160	ILE	-	expression tag	UNP Q8N1F7
B	161	GLU	-	expression tag	UNP Q8N1F7
B	162	TRP	-	expression tag	UNP Q8N1F7
B	163	HIS	-	expression tag	UNP Q8N1F7
B	164	GLU	-	expression tag	UNP Q8N1F7
B	165	GLY	-	expression tag	UNP Q8N1F7
B	166	SER	-	expression tag	UNP Q8N1F7
B	167	ALA	-	expression tag	UNP Q8N1F7
B	168	GLY	-	expression tag	UNP Q8N1F7
B	169	GLY	-	expression tag	UNP Q8N1F7
B	170	SER	-	expression tag	UNP Q8N1F7
B	171	GLY	-	expression tag	UNP Q8N1F7
B	172	GLY	-	expression tag	UNP Q8N1F7
B	173	SER	-	expression tag	UNP Q8N1F7

- Molecule 2 is a protein called Nucleoporin Nup35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	8	Total	C	H	N	O	0	0	0
			128	42	65	11	10			
2	C	8	Total	C	H	N	O	0	0	0
			128	42	65	11	10			

There are 2 discrepancies between the modelled and reference sequences:

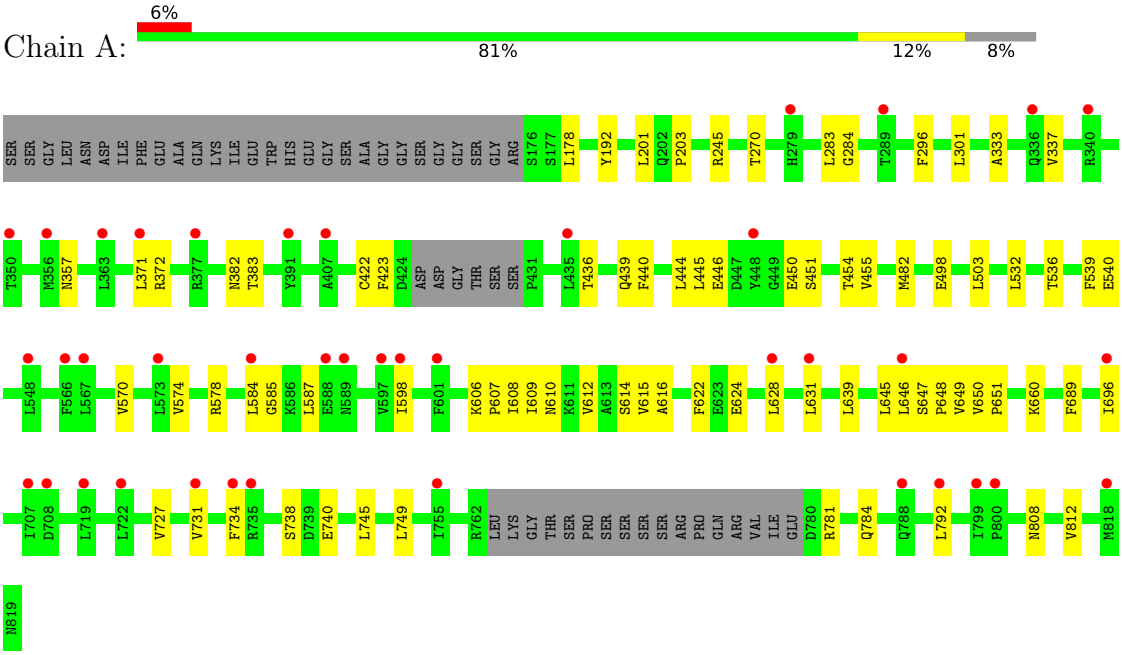
Chain	Residue	Modelled	Actual	Comment	Reference
D	83	SER	-	expression tag	UNP Q8NFH5
C	83	SER	-	expression tag	UNP Q8NFH5

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.

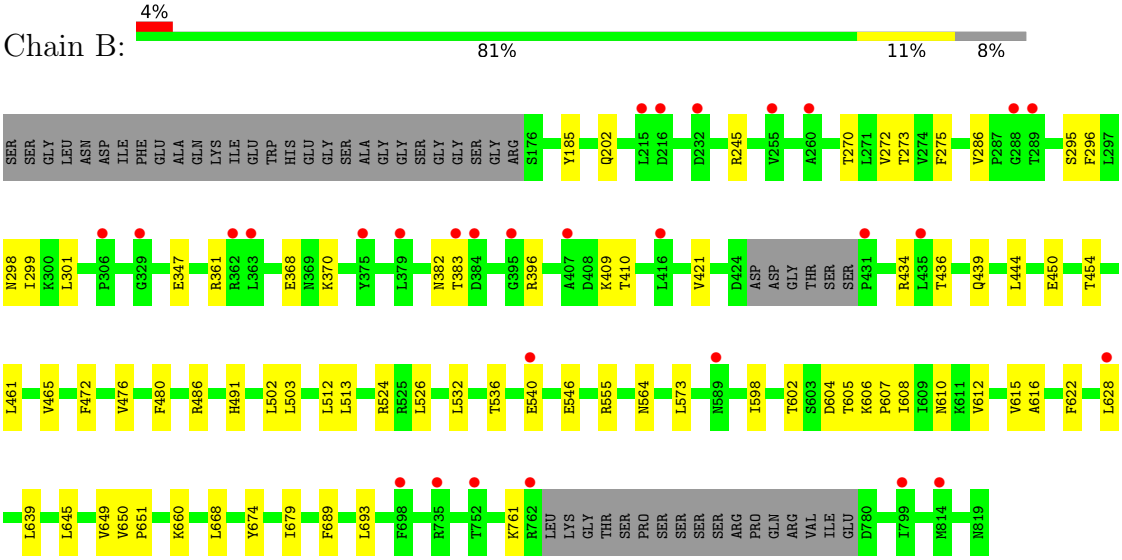
• Molecule 1: Nuclear pore complex protein Nup93

Chain A:



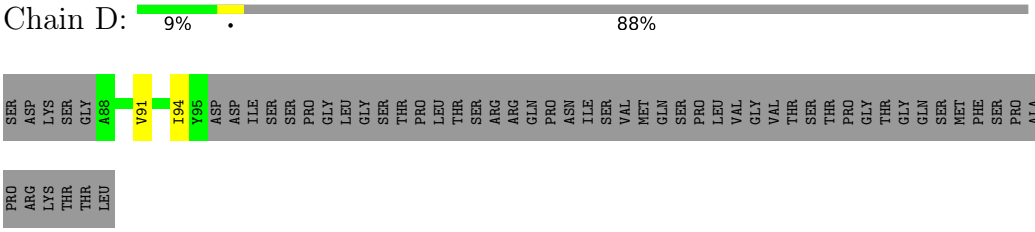
• Molecule 1: Nuclear pore complex protein Nup93

Chain B:



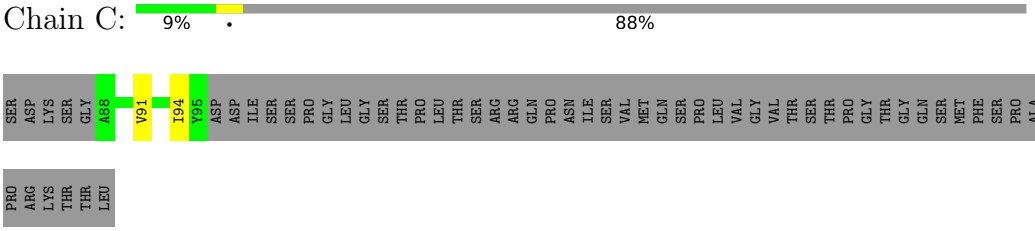
• Molecule 2: Nucleoporin Nup35

Chain D:



• Molecule 2: Nucleoporin Nup35

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.69Å 181.44Å 78.94Å 90.00° 94.03° 90.00°	Depositor
Resolution (Å)	33.76 – 3.40 39.31 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.76-3.40) 98.8 (39.31-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.229 , 0.276 0.224 , 0.269	Depositor DCC
R_{free} test set	2011 reflections (7.79%)	wwPDB-VP
Wilson B-factor (Å^2)	135.8	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 89.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20384	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	0.27	0/5130	0.43	0/6930
1	B	0.27	0/5130	0.42	0/6930
2	C	0.24	0/65	0.42	0/89
2	D	0.24	0/65	0.35	0/89
All	All	0.27	0/10390	0.42	0/14038

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

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	5034	5030	5030	53	0
1	B	5034	5030	5030	48	0
2	C	63	65	65	2	0
2	D	63	65	65	2	0
All	All	10194	10190	10190	103	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 5.

All (103) 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:B:450:GLU:O	1:B:454:THR:HG22	1.80	0.82
1:A:301:LEU:HD12	1:A:301:LEU:O	1.81	0.81
1:B:301:LEU:HD12	1:B:301:LEU:O	1.82	0.79
1:A:283:LEU:HD12	1:A:284:GLY:N	2.01	0.74
1:B:622:PHE:HB2	1:B:645:LEU:HD21	1.73	0.70
1:A:178:LEU:HD21	1:A:539:PHE:CG	2.27	0.70
1:B:298:ASN:OD1	1:B:299:ILE:N	2.25	0.70
1:A:622:PHE:HB2	1:A:645:LEU:HD21	1.72	0.70
1:A:451:SER:O	1:A:455:VAL:HG13	1.92	0.69
1:A:578:ARG:NH2	1:A:624:GLU:OE1	2.26	0.68
1:A:622:PHE:CB	1:A:645:LEU:HD21	2.25	0.67
1:A:450:GLU:O	1:A:454:THR:HG22	1.97	0.64
1:B:546:GLU:N	1:B:546:GLU:OE1	2.31	0.64
1:B:606:LYS:O	1:B:610:ASN:ND2	2.31	0.63
1:B:649:VAL:HG11	1:B:660:LYS:HA	1.81	0.62
1:B:368:GLU:OE2	1:B:434:ARG:NH2	2.33	0.61
1:B:612:VAL:HG12	1:B:628:LEU:HD13	1.81	0.61
1:B:461:LEU:O	1:B:465:VAL:HG23	2.01	0.61
1:A:270:THR:HG23	1:A:296:PHE:CD1	2.36	0.60
1:B:347:GLU:OE1	1:B:370:LYS:NZ	2.34	0.60
1:A:649:VAL:HG12	1:A:649:VAL:O	2.00	0.59
1:B:602:THR:HG22	1:B:604:ASP:H	1.67	0.59
1:A:570:VAL:HG11	1:A:598:ILE:HD12	1.86	0.58
1:A:598:ILE:HD13	1:A:608:ILE:CD1	2.34	0.58
1:B:649:VAL:O	1:B:649:VAL:HG12	2.04	0.57
1:A:738:SER:OG	1:A:740:GLU:OE1	2.22	0.57
2:D:91:VAL:O	2:D:91:VAL:HG22	2.04	0.57
2:C:91:VAL:HG22	2:C:91:VAL:O	2.04	0.57
1:A:201:LEU:O	1:A:203:PRO:HD3	2.05	0.57
1:A:585:GLY:O	1:A:631:LEU:HD11	2.06	0.56
1:B:674:TYR:CD1	1:B:679:ILE:HD11	2.42	0.55
1:A:612:VAL:HG12	1:A:628:LEU:HD13	1.88	0.55
1:B:185:TYR:HB3	1:B:491:HIS:NE2	2.21	0.54
1:A:532:LEU:O	1:A:536:THR:HG23	2.08	0.54
1:A:440:PHE:O	1:A:444:LEU:HD13	2.08	0.53
1:B:502:LEU:HD11	1:B:526:LEU:HD23	1.91	0.53
1:A:610:ASN:O	1:A:614:SER:N	2.43	0.52
1:A:649:VAL:HG11	1:A:660:LYS:HA	1.92	0.51
1:A:371:LEU:HD12	1:A:372:ARG:N	2.26	0.51
1:A:606:LYS:N	1:A:607:PRO:CD	2.74	0.50
1:A:646:LEU:HD22	1:A:696:ILE:CD1	2.42	0.50
1:B:606:LYS:N	1:B:607:PRO:CD	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LEU:HD22	1:A:689:PHE:CG	2.47	0.50
1:A:727:VAL:O	1:A:731:VAL:HG23	2.12	0.49
1:B:298:ASN:OD1	1:B:299:ILE:HG13	2.13	0.49
1:B:540:GLU:O	1:B:573:LEU:HD11	2.13	0.49
1:A:333:ALA:O	1:A:337:VAL:HG23	2.13	0.48
1:A:808:ASN:O	1:A:812:VAL:HG23	2.13	0.48
1:B:270:THR:HG23	1:B:296:PHE:CG	2.48	0.48
1:B:532:LEU:O	1:B:536:THR:HG23	2.13	0.48
1:B:409:LYS:HD3	2:D:94:ILE:HG22	1.95	0.48
1:B:436:THR:HG23	1:B:439:GLN:H	1.79	0.48
1:A:639:LEU:HD22	1:A:689:PHE:CD2	2.50	0.47
1:B:202:GLN:O	1:B:202:GLN:HG3	2.15	0.47
1:B:650:VAL:HB	1:B:651:PRO:HD3	1.97	0.47
1:B:396:ARG:NH1	1:B:421:VAL:O	2.47	0.47
1:B:273:THR:HG21	1:B:296:PHE:CE1	2.49	0.47
1:A:422:CYS:SG	1:A:423:PHE:N	2.88	0.47
1:A:615:VAL:HG23	1:A:616:ALA:N	2.29	0.46
1:B:615:VAL:HG23	1:B:616:ALA:N	2.30	0.46
1:B:622:PHE:CB	1:B:645:LEU:HD21	2.44	0.46
1:B:295:SER:HA	1:B:298:ASN:ND2	2.31	0.46
1:A:440:PHE:CE1	1:A:444:LEU:HD11	2.50	0.46
1:B:639:LEU:HD22	1:B:689:PHE:CG	2.50	0.46
1:B:605:THR:HG22	1:B:605:THR:O	2.16	0.46
1:B:361:ARG:O	1:B:396:ARG:NH2	2.45	0.46
1:B:480:PHE:O	1:B:486:ARG:NH1	2.49	0.46
1:B:555:ARG:O	1:B:564:ASN:ND2	2.46	0.46
1:B:444:LEU:HD23	1:B:465:VAL:CG1	2.45	0.45
1:B:639:LEU:HD22	1:B:689:PHE:CD2	2.51	0.45
1:A:436:THR:HG23	1:A:439:GLN:H	1.82	0.45
1:A:357:ASN:OD1	1:B:761:LYS:NZ	2.46	0.45
1:B:668:LEU:CD2	1:B:693:LEU:HD22	2.47	0.45
1:A:482:MET:N	1:A:482:MET:SD	2.90	0.45
1:A:781:ARG:NH1	1:A:784:GLN:OE1	2.49	0.45
1:A:192:TYR:OH	1:A:498:GLU:OE1	2.33	0.45
1:B:472:PHE:O	1:B:476:VAL:HG23	2.16	0.45
1:B:513:LEU:HD21	1:B:524:ARG:NE	2.32	0.45
1:A:646:LEU:HD22	1:A:696:ILE:HD11	1.98	0.45
1:B:245:ARG:HG3	1:B:503:LEU:HD21	1.99	0.45
1:A:382:ASN:OD1	1:A:383:THR:N	2.50	0.44
1:B:410:THR:HG21	1:B:461:LEU:HD11	1.98	0.44
1:B:512:LEU:O	1:B:526:LEU:HD12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:HD12	1:A:446:GLU:N	2.33	0.44
1:A:650:VAL:HB	1:A:651:PRO:HD3	1.99	0.44
1:B:598:ILE:HG12	1:B:608:ILE:HD11	1.99	0.43
1:A:649:VAL:HG12	1:A:660:LYS:HD2	2.01	0.43
1:A:587:LEU:HD13	1:A:631:LEU:HA	1.99	0.43
1:B:272:VAL:HA	1:B:275:PHE:O	2.18	0.43
1:A:445:LEU:HD12	1:A:445:LEU:C	2.39	0.43
1:A:584:LEU:HD22	1:A:609:ILE:CD1	2.49	0.43
1:A:749:LEU:CD2	1:A:792:LEU:HD22	2.48	0.42
1:B:382:ASN:OD1	1:B:383:THR:N	2.52	0.42
1:A:584:LEU:HD22	1:A:609:ILE:HD11	2.00	0.42
2:C:94:ILE:O	2:C:94:ILE:HG23	2.19	0.42
1:A:570:VAL:O	1:A:574:VAL:HG23	2.20	0.42
1:A:649:VAL:O	1:A:649:VAL:CG1	2.68	0.41
1:A:734:PHE:CE1	1:A:745:LEU:HD22	2.55	0.41
1:A:245:ARG:HG3	1:A:503:LEU:HD21	2.03	0.41
1:A:647:SER:HB3	1:A:648:PRO:HD3	2.03	0.41
1:A:606:LYS:N	1:A:607:PRO:HD2	2.36	0.40
1:B:286:VAL:O	1:B:286:VAL:HG23	2.22	0.40
1:A:536:THR:O	1:A:540:GLU:HB3	2.22	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	615/672 (92%)	604 (98%)	11 (2%)	0	100	100
1	B	615/672 (92%)	601 (98%)	14 (2%)	0	100	100
2	C	6/68 (9%)	6 (100%)	0	0	100	100
2	D	6/68 (9%)	6 (100%)	0	0	100	100
All	All	1242/1480 (84%)	1217 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	554/594 (93%)	554 (100%)	0	100	100
1	B	554/594 (93%)	554 (100%)	0	100	100
2	C	7/59 (12%)	7 (100%)	0	100	100
2	D	7/59 (12%)	7 (100%)	0	100	100
All	All	1122/1306 (86%)	1122 (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. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 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	621/672 (92%)	0.47	40 (6%) 19 20	108, 147, 187, 211	0
1	B	621/672 (92%)	0.49	29 (4%) 31 31	101, 136, 177, 194	0
2	C	8/68 (11%)	0.24	0 100 100	146, 156, 158, 163	0
2	D	8/68 (11%)	0.02	0 100 100	125, 143, 153, 167	0
All	All	1258/1480 (85%)	0.48	69 (5%) 25 25	101, 142, 182, 211	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	722	LEU	4.4
1	B	215	LEU	3.7
1	A	377	ARG	3.6
1	A	601	PHE	3.6
1	B	383	THR	3.5
1	A	734	PHE	3.4
1	A	735	ARG	3.2
1	A	707	ILE	3.1
1	B	216	ASP	3.0
1	B	384	ASP	3.0
1	A	628	LEU	3.0
1	B	431	PRO	2.9
1	A	589	ASN	2.9
1	A	631	LEU	2.8
1	B	306	PRO	2.8
1	A	598	ILE	2.7
1	B	752	THR	2.7
1	B	416	LEU	2.7
1	B	289	THR	2.7
1	A	719	LEU	2.6
1	A	363	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	435	LEU	2.6
1	A	289	THR	2.6
1	B	363	LEU	2.6
1	A	646	LEU	2.6
1	A	800	PRO	2.5
1	A	548	LEU	2.5
1	B	407	ALA	2.5
1	A	588	GLU	2.5
1	A	371	LEU	2.5
1	A	573	LEU	2.5
1	B	589	ASN	2.5
1	B	799	ILE	2.5
1	A	340	ARG	2.5
1	A	448	TYR	2.4
1	B	255	VAL	2.4
1	B	735	ARG	2.4
1	A	391	TYR	2.4
1	A	708	ASP	2.4
1	B	698	PHE	2.4
1	B	288	GLY	2.4
1	A	584	LEU	2.4
1	B	379	LEU	2.4
1	B	329	GLY	2.3
1	A	792	LEU	2.3
1	B	628	LEU	2.3
1	A	350	THR	2.3
1	B	395	GLY	2.3
1	A	788	GLN	2.3
1	A	818	MET	2.3
1	B	375	TYR	2.2
1	A	696	ILE	2.2
1	B	435	LEU	2.2
1	A	731	VAL	2.2
1	A	799	ILE	2.2
1	A	356	MET	2.2
1	A	755	ILE	2.2
1	A	336	GLN	2.2
1	B	362	ARG	2.1
1	B	762	ARG	2.1
1	B	232	ASP	2.1
1	A	279	HIS	2.1
1	A	566	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	597	VAL	2.1
1	B	814	MET	2.0
1	B	540	GLU	2.0
1	A	407	ALA	2.0
1	A	567	LEU	2.0
1	B	260	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 monosaccharides 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.