W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:29 AM GMT

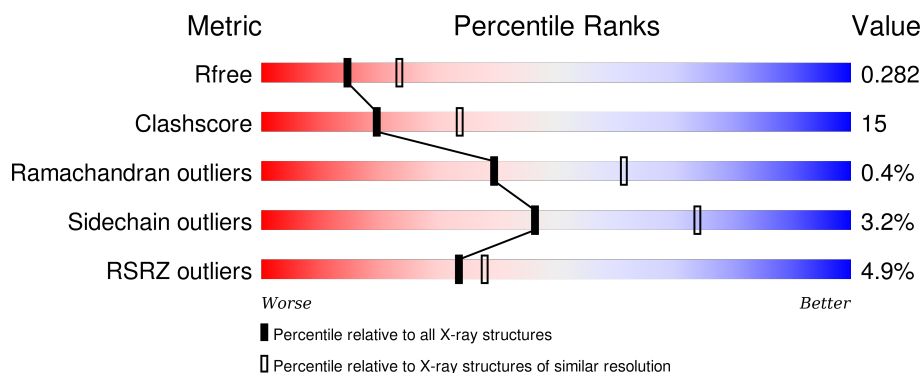|		
PDB ID	:	2QX5
Title	:	Structure of nucleoporin Nic96
Authors	:	Jeudy, S.; Schwartz, T.U.
Deposited on	:	2007-08-10
Resolution	:	2.50 Å(reported)

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1 Overall quality at a glance (i)

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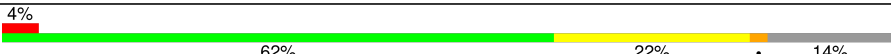*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.282
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		3.2%
RSRZ outliers		4.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	661	4% / 62% / 22% / • / 14%
1	B	661	4% / 62% / 22% / • / 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9160 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 Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4521	2910	752	842	17			
1	B	569	Total	C	N	O	S	0	0	0
			4514	2896	754	847	17			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	PRO	-	EXPRESSION TAG	UNP P34077
A	180	GLY	-	EXPRESSION TAG	UNP P34077
A	181	SER	-	EXPRESSION TAG	UNP P34077
A	182	GLU	-	EXPRESSION TAG	UNP P34077
A	183	PHE	-	EXPRESSION TAG	UNP P34077
A	184	GLU	-	EXPRESSION TAG	UNP P34077
A	185	LEU	-	EXPRESSION TAG	UNP P34077
B	179	PRO	-	EXPRESSION TAG	UNP P34077
B	180	GLY	-	EXPRESSION TAG	UNP P34077
B	181	SER	-	EXPRESSION TAG	UNP P34077
B	182	GLU	-	EXPRESSION TAG	UNP P34077
B	183	PHE	-	EXPRESSION TAG	UNP P34077
B	184	GLU	-	EXPRESSION TAG	UNP P34077
B	185	LEU	-	EXPRESSION TAG	UNP P34077

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	60	Total 60	O 60	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Nucleoporin NIC96
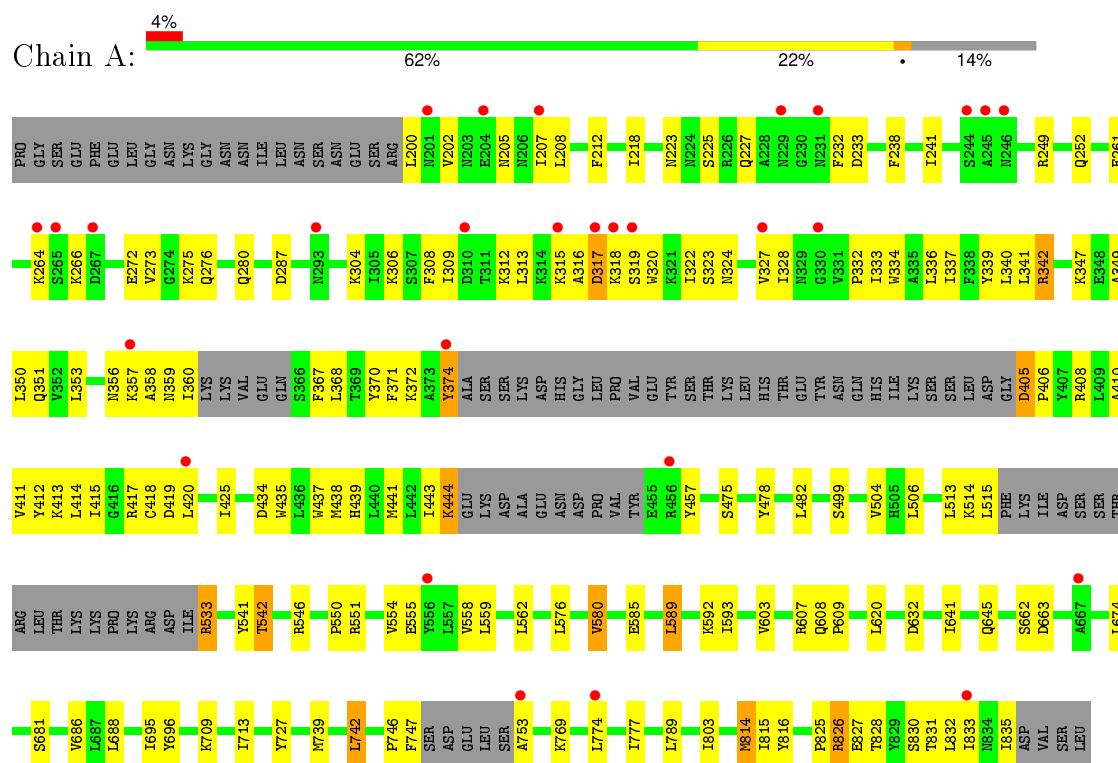
- Molecule 1: Nucleoporin NIC96
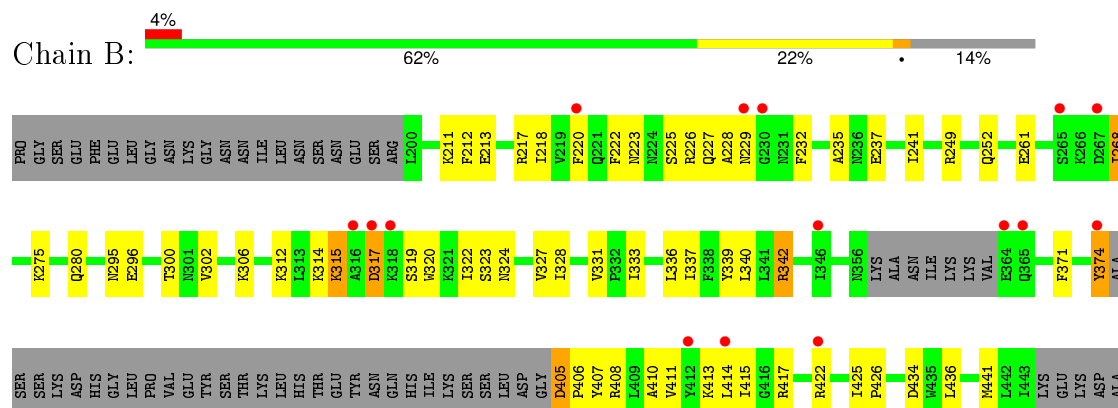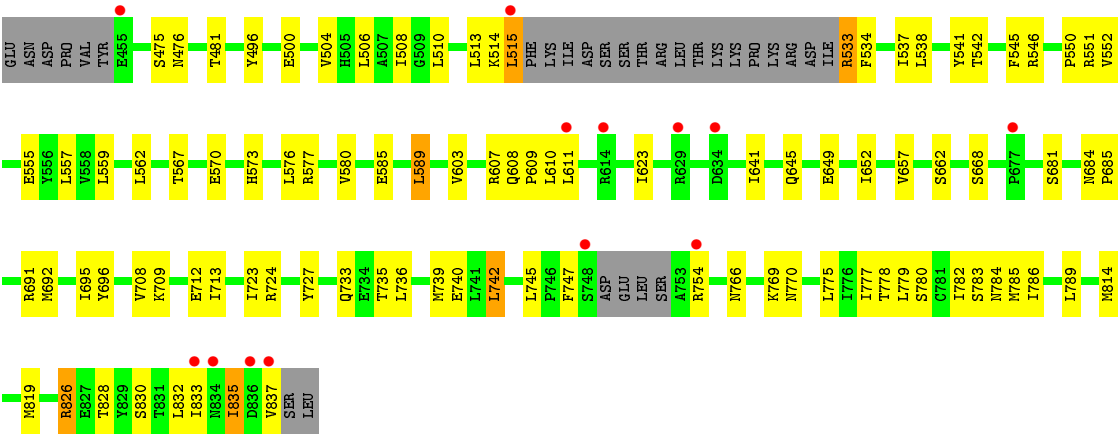
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.12Å　　82.48Å　　113.03Å 90.00°　　91.11°　　90.00°	Depositor
Resolution (Å)	20.00　−　2.50 32.08　−　2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.50) 98.3 (32.08-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$<I/\sigma(I)>$ [1]	4.41 (at 2.39Å)	Xtriage
Refinement program	phenix	Depositor
R, R_{free}	0.233　,　0.285 0.229　,　0.282	Depositor DCC
R_{free} test set	2761 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Outliers	8 of 61613 reflections (0.013%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0839e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.35	0/4597	0.50	0/6227
1	B	0.35	0/4590	0.51	0/6222
All	All	0.35	0/9187	0.50	0/12449

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	315	LYS	Peptide

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	4521	0	4530	133	0
1	B	4514	0	4486	138	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	63	0	0	3	0
3	B	60	0	0	6	0
All	All	9160	0	9016	271	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 15.

All (271) 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:533:ARG:HH11	1:B:533:ARG:HB2	1.07	1.15
1:A:357:LYS:O	1:A:360:ILE:HG12	1.46	1.12
1:A:533:ARG:HH11	1:A:533:ARG:HB2	0.96	1.11
1:B:533:ARG:HH11	1:B:533:ARG:CB	1.64	1.10
1:A:533:ARG:NH1	1:A:533:ARG:HB2	1.72	1.03
1:B:405:ASP:OD1	1:B:406:PRO:HD2	1.62	0.99
1:B:740:GLU:HG2	1:B:747:PHE:CE2	1.99	0.97
1:B:220:PHE:HD1	1:B:555:GLU:HG2	1.31	0.96
1:A:826:ARG:HG3	1:A:826:ARG:HH11	1.30	0.95
1:A:533:ARG:CB	1:A:533:ARG:HH11	1.81	0.93
1:B:533:ARG:NH1	1:B:533:ARG:HB2	1.83	0.93
1:B:220:PHE:CD1	1:B:555:GLU:HG2	2.05	0.92
1:B:374:TYR:HD2	1:B:374:TYR:C	1.74	0.91
1:B:649:GLU:HG2	1:B:652:ILE:HD12	1.53	0.89
1:B:826:ARG:HG3	1:B:826:ARG:HH11	1.38	0.86
1:B:374:TYR:CD2	1:B:374:TYR:C	2.45	0.86
1:A:825:PRO:HG2	1:A:828:THR:HG23	1.55	0.86
1:A:341:LEU:HD11	1:A:415:ILE:HD11	1.58	0.85
1:B:733:GLN:HG3	3:B:871:HOH:O	1.76	0.85
1:A:374:TYR:HD2	1:A:374:TYR:C	1.79	0.84
1:A:374:TYR:C	1:A:374:TYR:CD2	2.50	0.83
1:B:218:ILE:HD11	1:B:241:ILE:HD12	1.62	0.81
1:A:554:VAL:HG11	1:A:603:VAL:HG12	1.63	0.81
1:B:740:GLU:HG2	1:B:747:PHE:CD2	2.16	0.80
1:B:736:LEU:O	1:B:740:GLU:HG3	1.82	0.80
1:A:309:ILE:HG23	1:A:313:LEU:HD12	1.65	0.78
1:B:649:GLU:CG	1:B:652:ILE:HD12	2.14	0.77
1:B:786:ILE:HD12	1:B:837:VAL:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASP:OD1	1:B:406:PRO:CD	2.34	0.76
1:B:551:ARG:HG2	1:B:603:VAL:HG21	1.67	0.76
1:B:709:LYS:HE3	1:B:713:ILE:HD11	1.68	0.76
1:B:782:ILE:HG22	1:B:837:VAL:HG21	1.67	0.75
1:B:533:ARG:HH11	1:B:533:ARG:CG	1.97	0.75
1:B:249:ARG:HH11	1:B:252:GLN:HE22	1.37	0.73
1:A:353:LEU:HD23	1:A:368:LEU:HD13	1.71	0.73
1:B:573:HIS:O	1:B:577:ARG:HG3	1.88	0.73
1:A:264:LYS:HG2	1:A:513:LEU:HD21	1.71	0.72
1:A:357:LYS:O	1:A:360:ILE:CG1	2.34	0.71
1:A:826:ARG:CG	1:A:826:ARG:HH11	2.02	0.71
1:A:825:PRO:HG2	1:A:828:THR:CG2	2.21	0.70
1:A:405:ASP:HB2	1:A:406:PRO:HD2	1.72	0.70
1:A:218:ILE:HD11	1:A:241:ILE:HD12	1.72	0.70
1:A:662:SER:OG	1:A:769:LYS:HE2	1.93	0.69
1:A:641:ILE:O	1:A:645:GLN:HG3	1.92	0.69
1:A:275:LYS:HE3	1:A:441:MET:HE1	1.73	0.68
1:B:405:ASP:O	1:B:408:ARG:N	2.26	0.68
1:A:434:ASP:O	1:A:438:MET:HG2	1.93	0.68
1:A:370:TYR:CE2	1:A:415:ILE:HG22	2.29	0.67
1:B:405:ASP:OD1	1:B:405:ASP:C	2.34	0.66
1:B:826:ARG:CG	1:B:826:ARG:HH11	2.07	0.66
1:A:815:ILE:HG13	1:A:816:TYR:N	2.09	0.66
1:B:641:ILE:O	1:B:645:GLN:HG3	1.96	0.66
1:A:827:GLU:O	1:A:831:THR:HG23	1.96	0.65
1:B:227:GLN:NE2	1:B:607:ARG:HH11	1.94	0.65
1:A:333:ILE:O	1:A:337:ILE:HG13	1.97	0.64
1:A:334:TRP:CE2	1:A:408:ARG:HG3	2.32	0.64
1:A:515:LEU:O	1:A:515:LEU:HD12	1.97	0.64
1:A:317:ASP:HB2	1:A:319:SER:OG	1.98	0.64
1:B:783:SER:HA	1:B:837:VAL:HG23	1.79	0.64
1:B:786:ILE:HD12	1:B:837:VAL:CG2	2.28	0.62
1:B:300:THR:HG22	1:B:302:VAL:N	2.14	0.62
1:A:443:ILE:HG22	1:A:444:LYS:HG2	1.79	0.62
1:A:559:LEU:O	1:A:562:LEU:HB2	1.99	0.62
1:A:439:HIS:HD2	1:A:457:TYR:OH	1.82	0.62
1:A:320:TRP:CH2	1:A:332:PRO:HD3	2.34	0.62
1:A:832:LEU:O	1:A:835:ILE:HG22	2.00	0.61
1:B:533:ARG:NH1	1:B:533:ARG:CG	2.60	0.61
1:B:830:SER:O	1:B:833:ILE:HG22	2.00	0.61
1:A:342:ARG:NH1	1:A:434:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:TYR:CE2	1:B:500:GLU:HG3	2.36	0.61
1:B:410:ALA:O	1:B:414:LEU:HG	2.01	0.61
1:B:315:LYS:O	1:B:317:ASP:N	2.30	0.60
1:B:814:MET:HE2	1:B:814:MET:HA	1.82	0.60
1:A:264:LYS:HB2	1:A:264:LYS:NZ	2.17	0.60
1:B:317:ASP:N	1:B:317:ASP:OD1	2.33	0.60
1:A:350:LEU:HD11	1:A:372:LYS:HG2	1.84	0.60
1:A:315:LYS:O	1:A:316:ALA:HB3	2.02	0.60
1:B:405:ASP:O	1:B:407:TYR:N	2.36	0.59
1:B:550:PRO:HG2	1:B:585:GLU:HG3	1.84	0.58
1:B:227:GLN:HE22	1:B:607:ARG:HD3	1.68	0.58
1:A:592:LYS:HB3	1:A:592:LYS:NZ	2.18	0.58
1:A:413:LYS:NZ	1:A:419:ASP:HB3	2.17	0.58
1:B:275:LYS:HD2	3:B:864:HOH:O	2.03	0.58
1:A:410:ALA:O	1:A:414:LEU:HG	2.04	0.58
1:A:309:ILE:HD11	1:A:336:LEU:HA	1.85	0.58
1:B:567:THR:O	1:B:570:GLU:HG2	2.04	0.58
1:A:709:LYS:HE3	1:A:713:ILE:HD11	1.86	0.57
1:B:220:PHE:HZ	1:B:552:VAL:HG22	1.69	0.57
1:A:826:ARG:NH1	1:A:826:ARG:HG3	2.12	0.57
1:B:708:VAL:O	1:B:712:GLU:HG3	2.04	0.57
1:B:218:ILE:HD11	1:B:241:ILE:CD1	2.34	0.56
1:A:249:ARG:HH11	1:A:252:GLN:HE22	1.53	0.56
1:B:542:THR:O	1:B:546:ARG:HG3	2.04	0.56
1:B:223:ASN:HD22	1:B:555:GLU:HG3	1.71	0.56
1:A:405:ASP:CB	1:A:406:PRO:HD2	2.35	0.56
1:A:709:LYS:O	1:A:713:ILE:HG12	2.06	0.56
1:A:202:VAL:HG11	1:A:212:PHE:CG	2.41	0.56
1:A:287:ASP:OD1	1:A:304:LYS:HD3	2.06	0.56
1:B:249:ARG:HH11	1:B:252:GLN:NE2	2.02	0.55
1:B:709:LYS:O	1:B:713:ILE:HG12	2.07	0.55
1:A:233:ASP:OD1	1:A:264:LYS:HE2	2.06	0.55
1:A:695:ILE:HG22	1:A:696:TYR:CD1	2.42	0.55
1:B:814:MET:CE	1:B:814:MET:HA	2.37	0.55
1:B:754:ARG:HG2	1:B:819:MET:HE1	1.87	0.55
1:A:746:PRO:HB3	1:A:753:ALA:HA	1.89	0.54
1:A:323:SER:O	1:A:324:ASN:HB2	2.07	0.54
1:A:275:LYS:HG2	1:A:441:MET:HE2	1.88	0.54
1:B:333:ILE:O	1:B:337:ILE:HG13	2.07	0.54
1:A:420:LEU:H	1:A:420:LEU:HD12	1.73	0.54
1:B:723:ILE:HG23	1:B:735:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ARG:NH1	1:B:252:GLN:HE22	2.04	0.53
1:B:342:ARG:NH1	1:B:434:ASP:OD1	2.41	0.53
1:B:223:ASN:HA	1:B:226:ARG:HD3	1.90	0.53
1:B:510:LEU:O	1:B:515:LEU:HB2	2.08	0.53
1:A:327:VAL:C	1:A:328:ILE:HD12	2.28	0.53
1:A:308:PHE:CE1	1:A:312:LYS:HG3	2.44	0.53
1:B:302:VAL:CG1	1:B:306:LYS:HE3	2.39	0.53
1:B:496:TYR:HE2	1:B:500:GLU:HG3	1.74	0.52
1:A:504:VAL:HG21	1:A:541:TYR:HB2	1.91	0.52
1:A:830:SER:O	1:A:833:ILE:HG22	2.09	0.52
1:A:370:TYR:HE2	1:A:415:ILE:HG22	1.73	0.52
1:B:782:ILE:HG22	1:B:837:VAL:CG2	2.38	0.52
1:A:367:PHE:HB2	1:A:412:TYR:CZ	2.45	0.52
1:A:261:GLU:HA	1:A:264:LYS:HE3	1.90	0.51
1:A:227:GLN:NE2	1:A:607:ARG:HH11	2.08	0.51
1:B:542:THR:HA	1:B:545:PHE:CE2	2.46	0.51
1:A:413:LYS:HD2	1:A:425:ILE:HD13	1.91	0.51
1:B:514:LYS:O	1:B:515:LEU:HD23	2.10	0.51
1:A:340:LEU:HD23	1:A:349:ALA:HA	1.93	0.50
1:A:327:VAL:O	1:A:328:ILE:HD12	2.11	0.50
1:B:577:ARG:NH2	1:B:623:ILE:HA	2.25	0.50
1:A:835:ILE:O	1:A:835:ILE:HG23	2.10	0.50
1:A:309:ILE:CD1	1:A:336:LEU:HA	2.41	0.50
1:B:300:THR:HG22	1:B:302:VAL:H	1.76	0.50
1:B:542:THR:HA	1:B:545:PHE:CZ	2.46	0.50
1:B:739:MET:O	1:B:742:LEU:HB2	2.11	0.50
1:B:322:ILE:HD11	1:B:407:TYR:HE1	1.76	0.50
1:B:695:ILE:HG22	1:B:696:TYR:CD1	2.47	0.50
1:A:232:PHE:HE1	3:A:903:HOH:O	1.94	0.50
1:B:580:VAL:HG12	1:B:589:LEU:HD23	1.94	0.49
1:A:592:LYS:HG2	1:A:593:ILE:N	2.27	0.49
1:A:347:LYS:O	1:A:351:GLN:HG3	2.13	0.49
1:B:826:ARG:CG	1:B:826:ARG:NH1	2.72	0.49
1:A:358:ALA:C	1:A:360:ILE:H	2.15	0.49
1:A:322:ILE:HD11	1:A:406:PRO:HG3	1.94	0.49
1:B:302:VAL:HG12	1:B:306:LYS:HE3	1.93	0.49
1:B:662:SER:OG	1:B:769:LYS:HE2	2.12	0.49
1:A:200:LEU:CD1	1:A:208:LEU:HD21	2.43	0.49
1:B:323:SER:O	1:B:324:ASN:HB2	2.13	0.48
1:A:316:ALA:C	1:A:318:LYS:H	2.16	0.48
1:B:336:LEU:O	1:B:340:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD22	1:A:371:PHE:HD2	1.77	0.48
1:A:478:TYR:CE2	1:A:482:LEU:HD11	2.47	0.48
1:A:789:LEU:HB2	1:A:803:ILE:HD11	1.95	0.48
1:A:550:PRO:CG	1:A:585:GLU:HG3	2.44	0.48
1:A:405:ASP:C	1:A:405:ASP:OD1	2.53	0.47
1:A:443:ILE:CG2	1:A:444:LYS:N	2.76	0.47
1:A:739:MET:O	1:A:742:LEU:HB2	2.14	0.47
1:B:324:ASN:O	1:B:405:ASP:HB2	2.15	0.47
1:A:576:LEU:O	1:A:580:VAL:HG13	2.14	0.47
1:B:213:GLU:O	1:B:217:ARG:HG3	2.13	0.47
1:B:328:ILE:O	1:B:331:VAL:HG12	2.14	0.47
1:A:674:LEU:HD13	1:A:686:VAL:HG21	1.97	0.47
1:A:368:LEU:O	1:A:368:LEU:HD12	2.15	0.47
1:B:745:LEU:HD13	1:B:775:LEU:HD23	1.95	0.47
1:A:417:ARG:O	1:A:420:LEU:HD11	2.14	0.47
1:B:657:VAL:HG21	1:B:692:MET:HG3	1.95	0.47
1:A:727:TYR:CD1	1:A:777:ILE:HG23	2.50	0.47
1:A:814:MET:HE1	1:A:833:ILE:HA	1.96	0.47
1:A:832:LEU:HD23	1:A:832:LEU:C	2.36	0.46
1:B:832:LEU:O	1:B:832:LEU:HD23	2.15	0.46
1:B:835:ILE:O	1:B:835:ILE:HG23	2.15	0.46
1:A:249:ARG:HH11	1:A:252:GLN:NE2	2.13	0.46
1:B:314:LYS:HE3	1:B:320:TRP:CH2	2.50	0.46
1:B:322:ILE:HG13	1:B:322:ILE:O	2.16	0.46
1:B:783:SER:HA	1:B:837:VAL:CG2	2.46	0.46
1:B:227:GLN:NE2	1:B:607:ARG:CD	2.79	0.46
1:B:533:ARG:O	1:B:537:ILE:HG13	2.15	0.46
1:A:826:ARG:NH1	1:A:826:ARG:CG	2.68	0.46
1:A:315:LYS:O	1:A:316:ALA:CB	2.62	0.46
1:A:306:LYS:NZ	3:A:867:HOH:O	2.48	0.46
1:A:826:ARG:HD2	1:A:826:ARG:HA	1.81	0.45
1:A:340:LEU:HB3	1:A:349:ALA:HB2	1.98	0.45
1:A:411:VAL:O	1:A:415:ILE:HG12	2.16	0.45
1:B:727:TYR:CD1	1:B:777:ILE:HG23	2.50	0.45
1:B:268:ILE:HG13	1:B:268:ILE:O	2.16	0.45
1:A:322:ILE:CD1	1:A:406:PRO:HG3	2.46	0.45
1:B:436:LEU:HD21	1:B:481:THR:HG23	1.97	0.45
1:B:223:ASN:OD1	1:B:226:ARG:NH1	2.50	0.45
1:A:832:LEU:O	1:A:835:ILE:CG2	2.63	0.45
1:B:295:ASN:O	1:B:296:GLU:C	2.55	0.45
1:B:417:ARG:HD2	3:B:894:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASN:HD22	1:A:555:GLU:HG3	1.82	0.45
1:A:554:VAL:O	1:A:558:VAL:HG23	2.15	0.44
1:A:444:LYS:N	1:A:457:TYR:O	2.48	0.44
1:A:550:PRO:HG2	1:A:585:GLU:HG3	2.00	0.44
1:B:225:SER:CB	1:B:232:PHE:HB2	2.48	0.44
1:B:513:LEU:O	1:B:514:LYS:HB2	2.18	0.44
1:B:475:SER:HB3	1:B:476:ASN:H	1.56	0.44
1:A:620:LEU:HD23	1:A:620:LEU:HA	1.80	0.44
1:A:663:ASP:OD1	1:A:769:LYS:HE3	2.18	0.44
1:A:342:ARG:HD2	1:A:437:TRP:CE3	2.53	0.44
1:A:515:LEU:O	1:A:515:LEU:CD1	2.65	0.44
1:B:228:ALA:O	1:B:229:ASN:HB3	2.18	0.43
1:A:272:GLU:O	1:A:276:GLN:HG3	2.18	0.43
1:B:740:GLU:HG2	1:B:747:PHE:CZ	2.50	0.43
1:A:312:LYS:O	1:A:313:LEU:HD23	2.19	0.43
1:A:580:VAL:HG12	1:A:589:LEU:HD23	2.00	0.43
1:A:218:ILE:HG21	1:A:238:PHE:CE1	2.53	0.43
1:A:266:LYS:HD2	1:A:273:VAL:HG22	2.01	0.43
1:B:832:LEU:HD23	1:B:832:LEU:C	2.40	0.43
1:B:212:PHE:CZ	1:B:552:VAL:HG11	2.54	0.43
1:B:441:MET:HE1	3:B:864:HOH:O	2.17	0.43
1:B:684:ASN:HA	1:B:685:PRO:HD3	1.74	0.43
1:A:747:PHE:N	1:A:747:PHE:CD1	2.87	0.42
1:B:211:LYS:HE3	3:B:846:HOH:O	2.18	0.42
1:A:562:LEU:HA	1:A:562:LEU:HD12	1.73	0.42
1:B:504:VAL:HG21	1:B:541:TYR:HB2	2.00	0.42
1:A:356:ASN:O	1:A:357:LYS:C	2.58	0.42
1:B:557:LEU:HA	1:B:557:LEU:HD23	1.78	0.42
1:B:413:LYS:NZ	1:B:422:ARG:O	2.42	0.42
1:B:405:ASP:O	1:B:406:PRO:C	2.58	0.42
1:B:562:LEU:HA	1:B:562:LEU:HD23	1.95	0.42
1:A:608:GLN:N	1:A:609:PRO:HD2	2.34	0.42
1:B:235:ALA:HB1	1:B:261:GLU:HB2	2.00	0.42
1:A:417:ARG:HE	1:A:417:ARG:HB2	1.66	0.42
1:B:668:SER:OG	1:B:724:ARG:NH2	2.48	0.42
1:A:551:ARG:HG2	1:A:603:VAL:HG21	2.02	0.42
1:B:577:ARG:CZ	1:B:623:ILE:HD13	2.50	0.42
1:A:435:TRP:CE2	1:A:439:HIS:CE1	3.08	0.42
1:A:608:GLN:N	1:A:609:PRO:CD	2.82	0.42
1:B:508:ILE:HG12	1:B:559:LEU:HD13	2.00	0.42
1:B:681:SER:HB3	1:B:691:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:VAL:HG13	1:B:415:ILE:HD13	2.02	0.42
1:A:339:TYR:HA	1:A:342:ARG:HB3	2.02	0.42
1:B:339:TYR:HA	1:B:342:ARG:HB3	2.01	0.42
1:B:785:MET:O	1:B:789:LEU:HG	2.19	0.42
1:A:542:THR:HG22	1:A:546:ARG:HD2	2.00	0.42
1:B:551:ARG:HD3	3:B:884:HOH:O	2.20	0.41
1:B:754:ARG:HG2	1:B:819:MET:CE	2.50	0.41
1:B:576:LEU:HD11	1:B:611:LEU:HD21	2.02	0.41
1:B:779:LEU:HD22	1:B:814:MET:HE1	2.02	0.41
1:B:580:VAL:HA	1:B:589:LEU:HD23	2.02	0.41
1:B:371:PHE:CD1	1:B:415:ILE:HG12	2.55	0.41
1:B:766:ASN:O	1:B:770:ASN:ND2	2.53	0.41
1:A:340:LEU:HD23	1:A:349:ALA:N	2.34	0.41
1:A:632:ASP:CB	3:A:909:HOH:O	2.68	0.41
1:B:534:PHE:CZ	1:B:538:LEU:HD11	2.55	0.41
1:B:775:LEU:O	1:B:779:LEU:HB2	2.20	0.41
1:A:420:LEU:HD12	1:A:420:LEU:N	2.35	0.41
1:A:227:GLN:HE22	1:A:607:ARG:HD3	1.85	0.41
1:A:225:SER:CB	1:A:232:PHE:HB2	2.50	0.41
1:A:774:LEU:HA	1:A:774:LEU:HD23	1.87	0.41
1:B:786:ILE:CD1	1:B:837:VAL:HG22	2.45	0.41
1:B:232:PHE:CZ	1:B:237:GLU:HG3	2.55	0.41
1:A:205:ASN:OD1	1:A:207:ILE:HB	2.20	0.41
1:B:220:PHE:CZ	1:B:552:VAL:HG22	2.52	0.41
1:B:739:MET:HG2	1:B:778:THR:OG1	2.20	0.41
1:A:356:ASN:O	1:A:358:ALA:N	2.55	0.40
1:A:513:LEU:O	1:A:514:LYS:HB2	2.20	0.40
1:B:607:ARG:HD2	1:B:610:LEU:HD12	2.02	0.40
1:B:322:ILE:HD11	1:B:407:TYR:CE1	2.53	0.40
1:B:227:GLN:HG3	1:B:610:LEU:HG	2.04	0.40
1:B:780:SER:O	1:B:784:ASN:ND2	2.54	0.40
1:B:608:GLN:N	1:B:609:PRO:HD2	2.36	0.40
1:B:222:PHE:O	1:B:226:ARG:HG3	2.20	0.40
1:B:327:VAL:C	1:B:328:ILE:HD12	2.42	0.40
1:A:340:LEU:HD23	1:A:349:ALA:CA	2.51	0.40
1:B:425:ILE:HA	1:B:426:PRO:HD3	1.84	0.40
1:A:357:LYS:O	1:A:360:ILE:CG2	2.68	0.40
1:A:742:LEU:HA	1:A:742:LEU:HD12	1.92	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	557/661 (84%)	537 (96%)	17 (3%)	3 (0%)	34	55
1	B	557/661 (84%)	533 (96%)	22 (4%)	2 (0%)	39	61
All	All	1114/1322 (84%)	1070 (96%)	39 (4%)	5 (0%)	39	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	835	ILE
1	A	317	ASP
1	A	499	SER
1	B	268	ILE
1	A	359	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	490/598 (82%)	473 (96%)	17 (4%)	43	70
1	B	489/598 (82%)	475 (97%)	14 (3%)	50	77
All	All	979/1196 (82%)	948 (97%)	31 (3%)	46	74

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	GLN

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Mol	Chain	Res	Type
1	A	342	ARG
1	A	374	TYR
1	A	405	ASP
1	A	418	CYS
1	A	444	LYS
1	A	475	SER
1	A	506	LEU
1	A	533	ARG
1	A	542	THR
1	A	580	VAL
1	A	589	LEU
1	A	681	SER
1	A	688	LEU
1	A	742	LEU
1	A	814	MET
1	A	826	ARG
1	B	280	GLN
1	B	312	LYS
1	B	317	ASP
1	B	319	SER
1	B	342	ARG
1	B	374	TYR
1	B	405	ASP
1	B	506	LEU
1	B	515	LEU
1	B	533	ARG
1	B	589	LEU
1	B	742	LEU
1	B	826	ARG
1	B	828	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	221	GLN
1	A	227	GLN
1	A	252	GLN
1	A	329	ASN
1	A	439	HIS
1	A	645	GLN
1	A	710	ASN

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Mol	Chain	Res	Type
1	A	766	ASN
1	A	812	GLN
1	A	834	ASN
1	B	206	ASN
1	B	221	GLN
1	B	227	GLN
1	B	229	ASN
1	B	252	GLN
1	B	324	ASN
1	B	329	ASN
1	B	439	HIS
1	B	710	ASN
1	B	731	GLN
1	B	766	ASN
1	B	773	ASN
1	B	834	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	569/661 (86%)	0.10	28 (4%)	33	38	31, 56, 100, 135	0
1	B	569/661 (86%)	0.13	28 (4%)	33	38	33, 58, 106, 143	0
All	All	1138/1322 (86%)	0.12	56 (4%)	33	38	31, 58, 102, 143	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	833	ILE	5.4
1	A	265	SER	4.9
1	B	316	ALA	4.6
1	B	267	ASP	4.3
1	B	754	ARG	4.1
1	A	231	ASN	3.6
1	A	245	ALA	3.6
1	B	265	SER	3.4
1	A	207	ILE	3.2
1	A	315	LYS	3.2
1	B	229	ASN	3.1
1	B	634	ASP	3.1
1	B	317	ASP	3.1
1	B	614	ARG	3.1
1	A	317	ASP	3.0
1	A	327	VAL	3.0
1	B	611	LEU	3.0
1	B	515	LEU	3.0
1	B	837	VAL	3.0
1	A	357	LYS	2.9
1	B	318	LYS	2.9
1	A	246	ASN	2.8
1	A	264	LYS	2.6
1	B	364	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	LYS	2.5
1	A	753	ALA	2.5
1	A	456	ARG	2.5
1	B	836	ASP	2.5
1	B	629	ARG	2.5
1	B	834	ASN	2.4
1	A	204	GLU	2.4
1	A	556	TYR	2.4
1	A	833	ILE	2.4
1	A	244	SER	2.4
1	A	229	ASN	2.4
1	A	667	ALA	2.4
1	B	230	GLY	2.3
1	A	774	LEU	2.3
1	B	677	PRO	2.3
1	A	420	LEU	2.2
1	B	346	ILE	2.2
1	B	220	PHE	2.2
1	B	365	GLN	2.2
1	B	455	GLU	2.2
1	A	374	TYR	2.2
1	A	267	ASP	2.2
1	B	422	ARG	2.2
1	B	414	LEU	2.1
1	A	293	ASN	2.1
1	B	748	SER	2.1
1	A	310	ASP	2.1
1	A	201	ASN	2.1
1	A	319	SER	2.1
1	B	374	TYR	2.1
1	A	330	GLY	2.1
1	B	412	TYR	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	B	844	1/1	0.94	0.25	1.09	57,57,57,57	0
2	CL	A	854	1/1	0.92	0.18	-0.33	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.