Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:00 am BST

PDB ID	:	2RFO
Title	:	Crystral Structure of the nucleoporin Nic96
Authors	:	Schrader, N.; Stelter, P.; Flemming, D.; Kunze, K.; Hurt, E.; Vetter, I.R.
Deposited on	:	2007-10-01
Resolution	:	2.60 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:

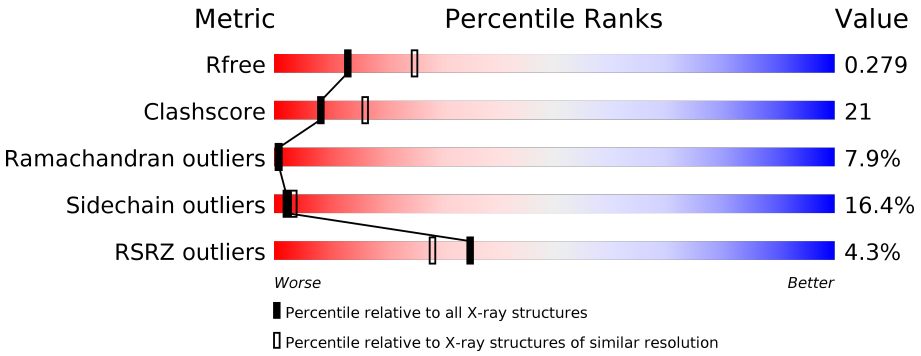
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	651	5% 55% 27% 10% • 6%
1	B	651	3% 50% 29% 12% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9984 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	612	Total	C	N	O	S	0	0	0
			4961	3171	836	937	17			
1	B	609	Total	C	N	O	S	0	0	0
			4935	3156	831	931	17			

- Molecule 2 is water.

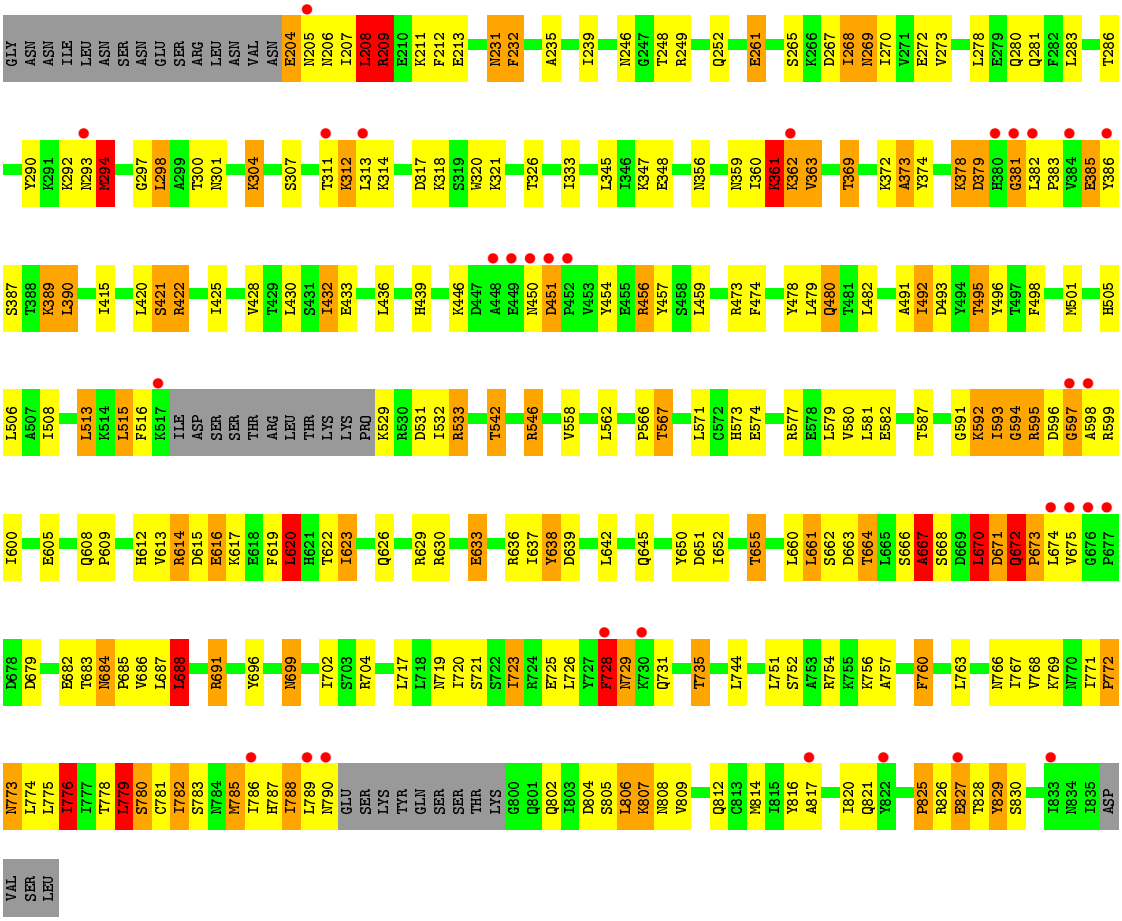
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	51	Total	O	0	0
			51	51		

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.

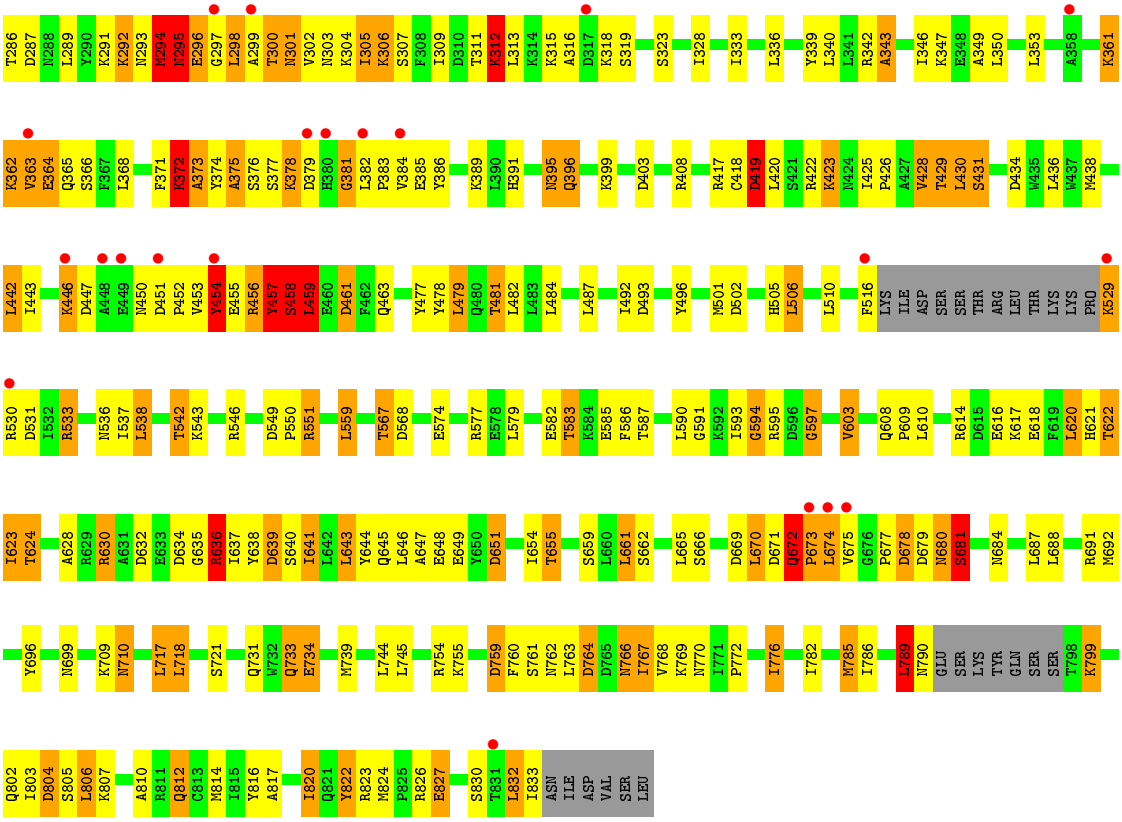
- Molecule 1: Nucleoporin NIC96

Chain A:



- Molecule 1: Nucleoporin NIC96

Chain B:


T286 D287 N288 L289 V290 K291 K292 N293 M294 N295 E296 G297 L298 A299 T300 N301 V302 N303 K304 I305 K306 S307 F308 I309 D310 T311 K312 L313 K314 K315 A316 D317 K318 S319 S323 I328 I333 L336 Y339 L340 L341 R342 A343 I346 K347 E348 A349 L350 L353 A358 K361
K362 V363 E364 Q365 S366 F367 L368 F371 K372 A373 Y374 A375 S376 S377 K378 D379 H380 G381 L382 P383 V384 E385 Y386 K389 L390 H391 N395 Q396 K399 D403 R408 R417 C418 D419 L420 S421 R422 K423 N424 I425 P426 A427 V428 T429 L430 S431 D434 W435 L436 W437 M438
L442 I443 K446 D447 A448 E449 N450 D451 P452 V453 Y454 E455 R456 Y457 S458 L459 E460 D461 F462 Q463 Y477 Y478 L479 Q480 T481 L482 L483 L484 L487 I492 D493 Y496 M501 D502 H505 L506 L510 F516 LYS ILE ASP SER SER THR ARG LEU THR LYS LYS PRO K529
R530 D531 I532 R533 N536 I537 L538 T542 K543 R546 D549 P550 R551 L559 T567 D568 E574 R577 E578 L579 E582 T583 K584 E585 F586 T587 L590 G591 K592 I593 G594 R595 D596 G597 V603 Q608 P609 L610 R614 D615 E616 K617 E618 F619 L620 H621 T622
I623 T624 A628 R629 R630 A631 D632 E633 D634 G635 R636 I637 Y638 D639 S640 I641 L642 L643 Y644 Q645 L646 A647 E648 E649 Y650 D651 I654 T655 S659 L660 L661 S662 L665 S666 D669 L670 D671 Q672 P673 L674 V675 G676 P677 D678 D679 N680 S681 N684 L687 L688 R691 M692
Y696 N699 K709 N710 L717 L718 S721 Q731 W732 Q733 E734 M739 L744 L745 R754 K755 D759 F760 S761 N762 L763 D764 D765 N766 I767 V768 K769 N770 T771 P772 I776 I782 M785 I786 L789 N790 GLU SER LYS TYR GLN SER SER T798 K799
Q802 I803 D804 S805 L806 K807 A810 R811 Q812 C813 M814 I815 Y816 A817 I820 Q821 Y822 R823 M824 P825 R826 E827 S830 T831 L832 I833 ASN ILE ASP VAL SER LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.00Å 100.00Å 104.00Å 62.00° 82.00° 86.00°	Depositor
Resolution (Å)	19.78 – 2.60 19.78 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.78-2.60) 78.9 (19.78-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.285 0.225 , 0.279	Depositor DCC
R_{free} test set	3313 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9984	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.63	3/5048 (0.1%)	0.77	6/6825 (0.1%)
1	B	1.31	19/5022 (0.4%)	0.86	8/6790 (0.1%)
All	All	1.03	22/10070 (0.2%)	0.81	14/13615 (0.1%)

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	A	0	5
1	B	0	4
All	All	0	9

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	GLU	CD-OE1	53.18	1.84	1.25
1	B	597	GLY	CA-C	34.73	2.07	1.51
1	B	296	GLU	CD-OE2	-26.74	0.96	1.25
1	B	296	GLU	CG-CD	19.24	1.80	1.51
1	B	636	ARG	CZ-NH1	17.23	1.55	1.33
1	B	790	ASN	CG-OD1	13.69	1.54	1.24
1	B	295	ASN	CG-OD1	13.08	1.52	1.24
1	B	296	GLU	CB-CG	11.94	1.74	1.52
1	B	597	GLY	N-CA	11.24	1.62	1.46
1	B	294	MET	CG-SD	9.42	2.05	1.81
1	B	678	ASP	CG-OD2	7.76	1.43	1.25
1	A	667	ALA	CA-CB	7.46	1.68	1.52
1	B	789	LEU	CG-CD1	7.05	1.77	1.51
1	A	297	GLY	C-O	6.57	1.34	1.23
1	B	295	ASN	CG-ND2	6.56	1.49	1.32
1	B	678	ASP	CG-OD1	6.13	1.39	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	MET	SD-CE	5.73	2.10	1.77
1	A	667	ALA	N-CA	5.63	1.57	1.46
1	B	790	ASN	CG-ND2	5.39	1.46	1.32
1	B	594	GLY	C-N	5.04	1.45	1.34
1	B	300	THR	CB-OG1	5.03	1.53	1.43
1	B	636	ARG	CD-NE	5.02	1.54	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	296	GLU	CG-CD-OE2	13.23	144.77	118.30
1	B	296	GLU	CG-CD-OE1	-11.73	94.85	118.30
1	B	636	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	B	419	ASP	CB-CG-OD1	-9.25	109.98	118.30
1	A	208	LEU	CA-CB-CG	8.16	134.06	115.30
1	B	597	GLY	N-CA-C	-7.99	93.12	113.10
1	B	458	SER	N-CA-C	6.62	128.87	111.00
1	A	688	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	513	LEU	CA-CB-CG	5.97	129.02	115.30
1	A	670	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	390	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	779	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	538	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	597	GLY	O-C-N	5.02	130.73	122.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	MET	Peptide
1	A	361	LYS	Peptide
1	A	599	ARG	Peptide
1	A	672	GLN	Peptide
1	A	728	PHE	Peptide
1	B	206	ASN	Peptide
1	B	456	ARG	Peptide
1	B	457	TYR	Peptide
1	B	458	SER	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	4961	0	5011	196	0
1	B	4935	0	4989	227	0
2	A	37	0	0	0	0
2	B	51	0	0	4	0
All	All	9984	0	10000	418	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 21.

All (418) 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:296:GLU:CB	1:B:296:GLU:CG	1.74	1.61
1:B:789:LEU:CD1	1:B:789:LEU:CG	1.77	1.61
1:B:296:GLU:CD	1:B:296:GLU:CG	1.80	1.49
1:B:294:MET:CG	1:B:294:MET:SD	2.05	1.44
1:B:294:MET:SD	1:B:294:MET:CE	2.09	1.40
1:B:597:GLY:CA	1:B:597:GLY:C	2.07	1.22
1:B:621:HIS:O	1:B:622:THR:HG22	1.37	1.20
1:B:296:GLU:CD	1:B:296:GLU:OE1	1.84	1.15
1:B:672:GLN:HB3	1:B:673:PRO:HD3	1.28	1.11
1:B:804:ASP:HA	1:B:807:LYS:HB2	1.31	1.09
1:A:682:GLU:HG3	1:A:688:LEU:HD23	1.36	1.06
1:A:663:ASP:O	1:A:664:THR:HG23	1.56	1.05
1:A:209:ARG:HH11	1:A:209:ARG:HG3	1.25	1.00
1:B:755:LYS:O	1:B:759:ASP:HB2	1.62	0.99
1:A:480:GLN:HE21	1:A:480:GLN:H	1.09	0.97
1:B:583:THR:HG23	1:B:585:GLU:H	1.35	0.92
1:B:672:GLN:HB3	1:B:673:PRO:CD	1.98	0.92
1:A:651:ASP:O	1:A:655:THR:HG22	1.71	0.89
1:A:805:SER:O	1:A:806:LEU:HB2	1.71	0.87
1:B:428:VAL:HG12	1:B:429:THR:H	1.39	0.87
1:B:505:HIS:O	1:B:506:LEU:CB	2.22	0.86
1:A:362:LYS:HA	1:A:362:LYS:HE3	1.57	0.84
1:B:595:ARG:HA	1:B:691:ARG:HH12	1.42	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:HIS:O	1:B:622:THR:CG2	2.24	0.83
1:A:619:PHE:O	1:A:620:LEU:HB2	1.79	0.82
1:B:812:GLN:HE21	1:B:812:GLN:HA	1.45	0.82
1:A:592:LYS:HG3	1:A:593:ILE:HG23	1.60	0.81
1:B:681:SER:HB3	1:B:691:ARG:HD3	1.61	0.81
1:B:692:MET:HE3	1:B:696:TYR:CE1	2.16	0.81
1:A:269:ASN:C	1:A:269:ASN:HD22	1.84	0.81
1:B:218:ILE:HD12	1:B:237:GLU:HG2	1.62	0.80
1:B:671:ASP:O	1:B:673:PRO:HD2	1.81	0.79
1:A:581:LEU:O	1:A:582:GLU:HG2	1.83	0.79
1:B:641:ILE:O	1:B:645:GLN:HG3	1.82	0.79
1:B:692:MET:CE	1:B:696:TYR:CE1	2.67	0.78
1:A:566:PRO:O	1:A:567:THR:HB	1.85	0.77
1:A:704:ARG:HH22	1:B:298:LEU:HG	1.49	0.77
1:B:594:GLY:O	1:B:597:GLY:N	2.17	0.77
1:B:206:ASN:O	1:B:207:ILE:HG23	1.84	0.77
1:B:428:VAL:HG12	1:B:429:THR:N	1.99	0.76
1:B:505:HIS:O	1:B:506:LEU:HB2	1.87	0.75
1:B:381:GLY:O	1:B:383:PRO:HD3	1.86	0.75
1:A:699:ASN:C	1:A:699:ASN:HD22	1.90	0.75
1:B:639:ASP:O	1:B:640:SER:HB3	1.87	0.75
1:A:752:SER:O	1:A:756:LYS:HG2	1.87	0.74
1:B:666:SER:HB2	1:B:769:LYS:HG3	1.69	0.74
1:A:378:LYS:NZ	1:A:378:LYS:HA	2.03	0.73
1:B:447:ASP:HA	1:B:450:ASN:HB2	1.70	0.73
1:A:300:THR:O	1:A:304:LYS:HD3	1.88	0.73
1:A:778:THR:O	1:A:782:ILE:HB	1.88	0.73
1:B:420:LEU:O	1:B:423:LYS:HD3	1.88	0.73
1:A:209:ARG:CG	1:A:209:ARG:HH11	2.00	0.72
1:B:587:THR:HA	1:B:591:GLY:O	1.90	0.72
1:B:293:ASN:OD1	1:B:295:ASN:HB2	1.89	0.72
1:A:205:ASN:HD22	1:A:208:LEU:HD13	1.56	0.71
1:A:663:ASP:O	1:A:664:THR:CG2	2.37	0.71
1:B:739:MET:HE1	1:B:745:LEU:HD22	1.73	0.71
1:A:491:ALA:O	1:A:495:THR:HG22	1.89	0.71
1:B:342:ARG:O	1:B:343:ALA:HB3	1.91	0.70
1:A:369:THR:O	1:A:372:LYS:O	2.09	0.70
1:B:595:ARG:HA	1:B:691:ARG:NH1	2.07	0.69
1:B:546:ARG:NH2	1:B:582:GLU:OE2	2.26	0.69
1:A:608:GLN:HB2	1:A:609:PRO:HD3	1.75	0.69
1:A:592:LYS:CG	1:A:593:ILE:HG23	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:LYS:NZ	1:B:770:ASN:H	1.89	0.68
1:B:256:SER:OG	1:B:479:LEU:HD13	1.94	0.67
1:A:312:LYS:HG3	1:A:313:LEU:H	1.57	0.67
1:A:278:LEU:HD22	1:A:433:GLU:HB2	1.76	0.67
1:B:769:LYS:HZ3	1:B:770:ASN:N	1.93	0.67
1:A:779:LEU:HD21	1:A:814:MET:HE1	1.76	0.67
1:B:212:PHE:N	1:B:501:MET:HE1	2.10	0.66
1:B:789:LEU:CD1	1:B:789:LEU:CB	2.72	0.66
1:A:615:ASP:O	1:A:617:LYS:N	2.27	0.66
1:B:789:LEU:CD2	1:B:789:LEU:CD1	2.72	0.66
1:A:425:ILE:CG2	1:A:428:VAL:HG22	2.26	0.66
1:B:477:TYR:O	1:B:481:THR:CG2	2.44	0.66
1:B:651:ASP:O	1:B:655:THR:HG23	1.95	0.66
1:B:769:LYS:HZ3	1:B:770:ASN:H	1.41	0.65
1:B:502:ASP:O	1:B:505:HIS:O	2.15	0.65
1:A:267:ASP:HB3	1:B:614:ARG:HH21	1.61	0.65
1:A:781:CYS:O	1:A:785:MET:HB2	1.96	0.64
1:B:628:ALA:HA	1:B:643:LEU:HD23	1.80	0.64
1:B:812:GLN:CA	1:B:812:GLN:HE21	2.09	0.64
1:A:372:LYS:O	1:A:373:ALA:CB	2.45	0.64
1:A:425:ILE:HG22	1:A:428:VAL:HG22	1.80	0.64
1:B:477:TYR:O	1:B:481:THR:HG23	1.98	0.64
1:B:505:HIS:O	1:B:506:LEU:HB3	1.96	0.64
1:A:827:GLU:O	1:A:827:GLU:HG2	1.97	0.64
1:A:660:LEU:O	1:A:664:THR:HG23	1.99	0.63
1:B:431:SER:HA	2:B:874:HOH:O	2.00	0.62
1:A:672:GLN:HE21	1:A:672:GLN:HA	1.65	0.62
1:A:731:GLN:O	1:A:735:THR:HG22	1.98	0.62
1:B:458:SER:HB2	1:B:461:ASP:HB2	1.81	0.62
1:A:211:LYS:C	1:A:501:MET:HE1	2.19	0.62
1:B:214:ASN:ND2	1:B:217:ARG:HH21	1.98	0.61
1:B:297:GLY:O	1:B:299:ALA:N	2.33	0.61
1:B:681:SER:HB2	1:B:688:LEU:HA	1.82	0.61
1:B:769:LYS:O	1:B:770:ASN:HB2	2.01	0.61
1:A:211:LYS:HG2	1:A:501:MET:HE1	1.81	0.61
1:A:209:ARG:NH1	1:A:209:ARG:HG3	2.04	0.61
1:B:211:LYS:C	1:B:501:MET:HE1	2.21	0.61
1:B:346:ILE:HD12	1:B:347:LYS:H	1.66	0.60
1:B:374:TYR:O	1:B:375:ALA:CB	2.49	0.60
1:B:574:GLU:OE1	1:B:577:ARG:NH1	2.34	0.60
1:A:721:SER:O	1:A:725:GLU:HG2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:LYS:HG3	1:B:618:GLU:H	1.64	0.60
1:B:640:SER:O	1:B:641:ILE:HG13	2.00	0.60
1:B:218:ILE:HD12	1:B:237:GLU:CG	2.31	0.60
1:A:767:ILE:C	1:A:769:LYS:H	2.04	0.60
1:B:374:TYR:O	1:B:375:ALA:HB3	2.02	0.60
1:B:739:MET:CE	1:B:745:LEU:HD22	2.31	0.60
1:B:417:ARG:NH1	1:B:442:LEU:O	2.35	0.60
1:B:364:GLU:C	1:B:366:SER:H	2.03	0.60
1:A:670:LEU:O	1:A:671:ASP:HB3	2.02	0.59
1:B:305:ILE:O	1:B:306:LYS:CB	2.50	0.59
1:B:567:THR:HG22	2:B:871:HOH:O	2.02	0.59
1:A:361:LYS:HG3	1:A:363:VAL:H	1.65	0.59
1:B:212:PHE:HA	1:B:501:MET:CE	2.32	0.59
1:A:614:ARG:HG2	1:A:614:ARG:O	2.03	0.59
1:A:637:ILE:O	1:A:638:TYR:HB2	2.03	0.59
1:B:816:TYR:O	1:B:817:ALA:HB3	2.03	0.59
1:A:239:ILE:HD11	1:A:261:GLU:HG2	1.85	0.59
1:B:681:SER:CB	1:B:691:ARG:HD3	2.30	0.59
1:B:674:LEU:N	1:B:674:LEU:HD13	2.18	0.59
1:B:263:MET:HG2	1:B:273:VAL:HG11	1.84	0.59
1:B:620:LEU:O	1:B:623:ILE:HG22	2.02	0.59
1:B:620:LEU:O	1:B:624:THR:HG23	2.01	0.58
1:A:231:ASN:H	1:A:231:ASN:ND2	2.00	0.58
1:A:356:ASN:HD22	1:A:359:ASN:HD22	1.50	0.58
1:A:776:ILE:H	1:A:779:LEU:HD22	1.68	0.58
1:B:478:TYR:CE1	1:B:482:LEU:HD11	2.38	0.58
1:B:212:PHE:HA	1:B:501:MET:HE3	1.84	0.58
1:B:311:THR:HG22	1:B:312:LYS:H	1.69	0.58
1:B:772:PRO:HG3	1:B:824:MET:HG3	1.85	0.58
1:A:595:ARG:NH1	1:A:691:ARG:HH12	2.02	0.58
1:A:704:ARG:NH2	1:B:298:LEU:HG	2.17	0.58
1:A:372:LYS:O	1:A:373:ALA:HB2	2.04	0.57
1:A:682:GLU:CG	1:A:688:LEU:HD23	2.23	0.57
1:B:456:ARG:HG3	1:B:457:TYR:N	2.19	0.57
1:B:311:THR:HG22	1:B:312:LYS:N	2.19	0.57
1:B:457:TYR:CD1	1:B:458:SER:HB2	2.38	0.57
1:B:458:SER:OG	1:B:459:LEU:N	2.37	0.57
1:B:408:ARG:HD3	2:B:884:HOH:O	2.05	0.57
1:B:455:GLU:HA	1:B:455:GLU:OE2	2.05	0.57
1:A:592:LYS:HD2	1:A:593:ILE:HG23	1.86	0.57
1:B:383:PRO:HG2	1:B:386:TYR:HD2	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASP:OD2	1:B:403:ASP:N	2.34	0.56
1:A:421:SER:O	1:A:422:ARG:C	2.43	0.56
1:A:208:LEU:O	1:A:209:ARG:HB2	2.04	0.56
1:A:480:GLN:H	1:A:480:GLN:NE2	1.91	0.56
1:A:619:PHE:O	1:A:620:LEU:CB	2.51	0.56
1:A:719:ASN:O	1:A:723:ILE:HG23	2.05	0.56
1:B:293:ASN:C	1:B:295:ASN:H	2.08	0.55
1:A:231:ASN:H	1:A:231:ASN:HD22	1.54	0.55
1:B:644:TYR:O	1:B:648:GLU:O	2.24	0.55
1:B:328:ILE:HG13	1:B:333:ILE:HD11	1.88	0.55
1:A:450:ASN:O	1:A:451:ASP:HB2	2.06	0.55
1:A:566:PRO:O	1:A:567:THR:CB	2.54	0.55
1:B:583:THR:HG23	1:B:585:GLU:N	2.16	0.55
1:A:776:ILE:HG22	1:A:830:SER:OG	2.07	0.55
1:A:209:ARG:NH1	1:A:213:GLU:OE2	2.40	0.55
1:A:439:HIS:HD2	1:A:457:TYR:OH	1.89	0.55
1:A:211:LYS:HG2	1:A:501:MET:CE	2.37	0.55
1:A:782:ILE:O	1:A:786:ILE:HG12	2.05	0.55
1:B:425:ILE:HD12	1:B:438:MET:SD	2.47	0.55
1:A:769:LYS:O	1:A:769:LYS:HG3	2.06	0.54
1:B:282:PHE:HD1	1:B:343:ALA:HB2	1.72	0.54
1:B:531:ASP:CG	1:B:536:ASN:HD22	2.10	0.54
1:B:372:LYS:O	1:B:373:ALA:CB	2.55	0.54
1:B:296:GLU:CD	1:B:296:GLU:CB	2.75	0.54
1:B:305:ILE:O	1:B:306:LYS:HB3	2.07	0.54
1:A:298:LEU:HD13	1:A:300:THR:HG23	1.89	0.54
1:B:830:SER:O	1:B:832:LEU:HD13	2.08	0.54
1:B:802:GLN:O	1:B:805:SER:HB3	2.07	0.54
1:A:211:LYS:O	1:A:501:MET:HE1	2.09	0.53
1:A:782:ILE:HD11	1:A:809:VAL:HB	1.90	0.53
1:B:802:GLN:O	1:B:806:LEU:HD22	2.08	0.53
1:A:505:HIS:HA	1:A:508:ILE:HD12	1.90	0.53
1:A:595:ARG:NH1	1:A:691:ARG:NH1	2.57	0.53
1:A:779:LEU:HD21	1:A:814:MET:CE	2.38	0.53
1:A:613:VAL:C	1:A:615:ASP:H	2.11	0.53
1:A:771:ILE:O	1:A:772:PRO:C	2.46	0.53
1:B:463:GLN:HB3	1:B:487:LEU:HD21	1.91	0.53
1:A:779:LEU:O	1:A:780:SER:HB2	2.09	0.53
1:B:342:ARG:O	1:B:343:ALA:CB	2.54	0.53
1:A:595:ARG:HH11	1:A:691:ARG:NH1	2.06	0.53
1:A:280:GLN:HA	1:A:280:GLN:NE2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LYS:HD2	1:A:617:LYS:N	2.23	0.52
1:A:636:ARG:O	1:A:639:ASP:HB2	2.09	0.52
1:B:227:GLN:HG2	1:B:610:LEU:HD21	1.91	0.52
1:A:592:LYS:CD	1:A:593:ILE:HG23	2.40	0.52
1:A:515:LEU:O	1:A:516:PHE:HB2	2.09	0.52
1:B:362:LYS:C	1:B:364:GLU:H	2.13	0.52
1:A:360:ILE:O	1:A:361:LYS:HB2	2.10	0.52
1:A:204:GLU:HG3	1:A:204:GLU:O	2.09	0.52
1:B:430:LEU:O	1:B:431:SER:O	2.28	0.52
1:A:814:MET:HA	1:A:814:MET:HE2	1.91	0.52
1:B:304:LYS:O	1:B:307:SER:HB3	2.10	0.52
1:B:391:HIS:O	1:B:395:ASN:HB2	2.10	0.52
1:B:430:LEU:O	1:B:434:ASP:HB2	2.10	0.52
1:A:378:LYS:HZ2	1:A:378:LYS:HA	1.75	0.51
1:B:207:ILE:HG13	1:B:208:LEU:N	2.25	0.51
1:A:790:ASN:H	1:A:790:ASN:HD22	1.57	0.51
1:B:458:SER:CB	1:B:461:ASP:HB2	2.40	0.51
1:B:639:ASP:O	1:B:640:SER:CB	2.54	0.51
1:A:378:LYS:HZ3	1:A:378:LYS:HA	1.76	0.51
1:B:339:TYR:O	1:B:342:ARG:O	2.28	0.51
1:B:635:GLY:O	1:B:637:ILE:HG13	2.11	0.51
1:A:269:ASN:C	1:A:269:ASN:ND2	2.58	0.51
1:A:767:ILE:O	1:A:769:LYS:N	2.44	0.51
1:B:301:ASN:H	1:B:304:LYS:HG3	1.75	0.51
1:B:492:ILE:HD11	1:B:510:LEU:HD12	1.93	0.51
1:B:674:LEU:HG	1:B:687:LEU:HD11	1.93	0.51
1:A:592:LYS:HG3	1:A:593:ILE:N	2.26	0.51
1:B:362:LYS:O	1:B:364:GLU:N	2.44	0.51
1:B:516:PHE:O	1:B:516:PHE:HD2	1.94	0.50
1:B:655:THR:HG22	1:B:710:ASN:OD1	2.11	0.50
1:A:249:ARG:HD2	1:A:498:PHE:CG	2.47	0.50
1:B:315:LYS:N	1:B:319:SER:O	2.43	0.50
1:B:669:ASP:CG	1:B:670:LEU:H	2.13	0.50
1:A:661:LEU:HD13	1:A:717:LEU:HB3	1.94	0.50
1:A:802:GLN:O	1:A:802:GLN:HG2	2.12	0.50
1:A:239:ILE:CD1	1:A:261:GLU:HG2	2.42	0.50
1:A:587:THR:HA	1:A:591:GLY:O	2.12	0.50
1:A:630:ARG:HA	1:A:633:GLU:HG3	1.93	0.50
1:B:661:LEU:HD13	1:B:717:LEU:HB3	1.93	0.50
1:A:235:ALA:HB1	1:A:261:GLU:HB3	1.94	0.50
1:A:290:TYR:C	1:A:292:LYS:H	2.13	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:LEU:HD21	1:B:721:SER:HB3	1.94	0.50
1:A:616:GLU:OE1	1:A:616:GLU:N	2.45	0.49
1:B:674:LEU:HA	1:B:677:PRO:HB2	1.94	0.49
1:B:632:ASP:C	1:B:634:ASP:H	2.15	0.49
1:B:353:LEU:HB3	1:B:368:LEU:HD23	1.95	0.49
1:A:314:LYS:O	1:A:320:TRP:HA	2.13	0.49
1:B:680:ASN:O	1:B:681:SER:HB3	2.12	0.49
1:A:312:LYS:HE2	1:A:313:LEU:HG	1.94	0.49
1:A:613:VAL:O	1:A:615:ASP:N	2.46	0.49
1:A:617:LYS:HA	1:A:617:LYS:HE3	1.95	0.49
1:A:828:THR:C	1:A:830:SER:H	2.14	0.49
1:B:477:TYR:O	1:B:481:THR:HG22	2.12	0.49
1:A:542:THR:O	1:A:546:ARG:HG2	2.13	0.48
1:A:361:LYS:HG3	1:A:363:VAL:N	2.28	0.48
1:B:637:ILE:O	1:B:638:TYR:HB2	2.13	0.48
1:B:679:ASP:O	1:B:681:SER:N	2.44	0.48
1:A:312:LYS:HG3	1:A:313:LEU:N	2.27	0.48
1:B:731:GLN:NE2	1:B:734:GLU:HB2	2.29	0.48
1:A:249:ARG:HD2	1:A:498:PHE:CD1	2.49	0.48
1:A:492:ILE:HA	1:A:495:THR:HG23	1.95	0.48
1:B:630:ARG:O	1:B:636:ARG:NH2	2.47	0.48
1:B:361:LYS:HE3	1:B:362:LYS:HE2	1.95	0.48
1:B:812:GLN:NE2	1:B:812:GLN:HA	2.23	0.48
1:B:300:THR:HB	1:B:304:LYS:HG3	1.95	0.48
1:A:608:GLN:CB	1:A:609:PRO:HD3	2.44	0.48
1:B:763:LEU:O	1:B:763:LEU:HG	2.14	0.48
1:A:662:SER:OG	1:A:766:ASN:O	2.32	0.48
1:A:307:SER:O	1:A:311:THR:HB	2.14	0.47
1:B:478:TYR:HA	1:B:481:THR:HG23	1.94	0.47
1:B:538:LEU:HD21	1:B:559:LEU:HB3	1.96	0.47
1:B:608:GLN:HB2	1:B:609:PRO:HD3	1.95	0.47
1:B:292:LYS:HD3	1:B:298:LEU:HD11	1.96	0.47
1:B:306:LYS:HA	1:B:309:ILE:HB	1.96	0.47
1:B:492:ILE:HD13	1:B:506:LEU:HD12	1.96	0.47
1:B:493:ASP:O	1:B:496:TYR:HB2	2.14	0.47
1:A:781:CYS:C	1:A:783:SER:H	2.17	0.47
1:B:311:THR:O	1:B:313:LEU:N	2.46	0.47
1:B:590:LEU:HD22	1:B:624:THR:HG22	1.95	0.47
1:A:720:ILE:O	1:A:723:ILE:HG13	2.15	0.47
1:A:492:ILE:HD12	1:A:496:TYR:CE1	2.49	0.47
1:A:573:HIS:CE1	1:A:613:VAL:HG23	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ILE:O	1:A:638:TYR:CB	2.62	0.47
1:B:456:ARG:HG3	1:B:457:TYR:H	1.80	0.47
1:B:443:ILE:HG12	1:B:458:SER:HB3	1.97	0.47
1:A:432:ILE:HD11	1:A:474:PHE:HD2	1.80	0.47
1:B:822:TYR:O	1:B:823:ARG:HB2	2.14	0.47
1:A:420:LEU:C	1:A:421:SER:O	2.51	0.47
1:A:778:THR:HG22	1:A:782:ILE:HD12	1.96	0.47
1:B:364:GLU:C	1:B:366:SER:N	2.67	0.46
1:B:375:ALA:C	1:B:377:SER:H	2.19	0.46
1:B:418:CYS:O	1:B:419:ASP:C	2.52	0.46
1:B:769:LYS:HD2	1:B:769:LYS:HA	1.77	0.46
1:B:772:PRO:HG3	1:B:824:MET:CG	2.45	0.46
1:B:820:ILE:O	1:B:820:ILE:CG2	2.63	0.46
1:A:782:ILE:HG23	1:A:782:ILE:O	2.15	0.46
1:B:733:GLN:HG2	1:B:785:MET:SD	2.55	0.46
1:A:231:ASN:N	1:A:231:ASN:ND2	2.61	0.46
1:A:666:SER:O	1:A:667:ALA:HB2	2.15	0.46
1:B:396:GLN:HA	1:B:396:GLN:NE2	2.29	0.46
1:B:766:ASN:HA	1:B:766:ASN:HD22	1.58	0.46
1:B:692:MET:CE	1:B:696:TYR:HE1	2.23	0.46
1:A:313:LEU:HB3	1:A:321:LYS:HZ2	1.80	0.46
1:A:531:ASP:OD1	1:A:533:ARG:NH1	2.49	0.46
1:A:699:ASN:ND2	1:A:699:ASN:C	2.62	0.46
1:A:760:PHE:HA	1:A:763:LEU:HD22	1.98	0.46
1:B:551:ARG:HB2	1:B:603:VAL:HG21	1.97	0.46
1:B:399:LYS:HE3	1:B:419:ASP:OD1	2.15	0.46
1:B:669:ASP:O	1:B:670:LEU:HD12	2.16	0.46
1:A:345:LEU:HB3	1:A:348:GLU:CG	2.46	0.45
1:A:595:ARG:HH11	1:A:691:ARG:HH12	1.63	0.45
1:B:672:GLN:O	1:B:674:LEU:N	2.45	0.45
1:A:671:ASP:O	1:A:672:GLN:HB2	2.17	0.45
1:B:207:ILE:HG13	1:B:208:LEU:H	1.81	0.45
1:B:597:GLY:N	1:B:597:GLY:C	2.70	0.45
1:B:760:PHE:C	1:B:762:ASN:H	2.19	0.45
1:A:492:ILE:CD1	1:A:496:TYR:HE1	2.29	0.45
1:A:670:LEU:O	1:A:671:ASP:CB	2.64	0.45
1:A:779:LEU:HA	1:A:782:ILE:CG2	2.47	0.45
1:A:728:PHE:O	1:A:729:ASN:HB2	2.16	0.45
1:A:684:ASN:HD21	1:A:687:LEU:HB2	1.82	0.45
1:A:804:ASP:HA	1:A:807:LYS:HD2	1.99	0.44
1:B:346:ILE:H	1:B:346:ILE:HG13	1.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:HD21	1:B:372:LYS:HG2	1.99	0.44
1:A:231:ASN:O	1:A:232:PHE:C	2.54	0.44
1:A:492:ILE:HG13	1:A:493:ASP:N	2.32	0.44
1:A:629:ARG:O	1:A:633:GLU:HG2	2.17	0.44
1:A:672:GLN:N	1:A:673:PRO:CD	2.80	0.44
1:B:239:ILE:HD11	1:B:258:LYS:HA	1.98	0.44
1:B:665:LEU:CB	1:B:770:ASN:HD21	2.29	0.44
1:A:381:GLY:O	1:A:383:PRO:HD3	2.17	0.44
1:B:673:PRO:HA	1:B:674:LEU:HD13	2.00	0.44
1:B:209:ARG:NH2	1:B:549:ASP:OD2	2.51	0.44
1:B:772:PRO:O	1:B:776:ILE:HG23	2.17	0.44
1:A:660:LEU:HG	1:A:685:PRO:HB3	1.98	0.44
1:B:298:LEU:C	1:B:300:THR:HG23	2.38	0.44
1:A:605:GLU:O	1:A:608:GLN:HG3	2.17	0.44
1:A:614:ARG:HH11	1:A:614:ARG:HG3	1.82	0.44
1:A:779:LEU:HA	1:A:782:ILE:HG22	2.00	0.44
1:B:296:GLU:CA	1:B:296:GLU:CG	2.83	0.44
1:A:567:THR:O	1:A:571:LEU:HG	2.18	0.44
1:A:775:LEU:HD13	1:A:817:ALA:HB2	2.00	0.44
1:B:531:ASP:OD1	1:B:533:ARG:HD3	2.18	0.44
1:A:581:LEU:O	1:A:582:GLU:CG	2.59	0.44
1:A:682:GLU:HA	1:A:688:LEU:HB2	2.00	0.44
1:A:666:SER:HA	1:A:773:ASN:OD1	2.18	0.44
1:A:808:ASN:O	1:A:812:GLN:HG2	2.18	0.44
1:B:396:GLN:HA	1:B:396:GLN:HE21	1.83	0.44
1:A:596:ASP:O	1:A:597:GLY:C	2.56	0.43
1:A:208:LEU:O	1:A:209:ARG:CB	2.66	0.43
1:B:300:THR:HB	1:B:304:LYS:CG	2.47	0.43
1:B:550:PRO:HG3	1:B:585:GLU:HG3	2.00	0.43
1:A:787:HIS:CG	1:A:787:HIS:O	2.71	0.43
1:B:785:MET:CE	1:B:785:MET:HA	2.49	0.43
1:B:799:LYS:HD3	1:B:799:LYS:HA	1.59	0.43
1:B:812:GLN:CA	1:B:812:GLN:NE2	2.79	0.43
1:A:663:ASP:C	1:A:664:THR:CG2	2.87	0.43
1:A:756:LYS:O	1:A:816:TYR:CE1	2.71	0.43
1:B:542:THR:HG21	2:B:882:HOH:O	2.18	0.43
1:B:767:ILE:O	1:B:769:LYS:O	2.36	0.43
1:B:666:SER:CB	1:B:769:LYS:HG3	2.43	0.43
1:A:645:GLN:HG2	1:A:696:TYR:OH	2.18	0.43
1:B:340:LEU:HB3	1:B:349:ALA:HB2	1.99	0.43
1:A:312:LYS:HA	1:A:312:LYS:HD2	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:TYR:CG	1:B:529:LYS:HA	2.53	0.43
1:B:665:LEU:HB2	1:B:770:ASN:HD21	1.84	0.43
1:A:425:ILE:CG2	1:A:428:VAL:CG2	2.96	0.43
1:A:626:GLN:HA	1:A:629:ARG:HE	1.84	0.43
1:B:315:LYS:HB3	1:B:316:ALA:H	1.66	0.43
1:A:268:ILE:HA	1:A:273:VAL:HG11	2.01	0.43
1:B:516:PHE:O	1:B:516:PHE:CD2	2.72	0.42
1:B:699:ASN:C	1:B:699:ASN:OD1	2.58	0.42
1:A:670:LEU:O	1:A:670:LEU:HD12	2.19	0.42
1:A:650:TYR:CE1	1:A:702:ILE:HG12	2.54	0.42
1:A:265:SER:HB2	1:B:609:PRO:HA	2.01	0.42
1:A:674:LEU:HD22	1:A:675:VAL:HG23	2.01	0.42
1:B:640:SER:O	1:B:641:ILE:CB	2.67	0.42
1:A:301:ASN:HB3	1:A:345:LEU:HD13	2.01	0.42
1:B:680:ASN:O	1:B:681:SER:CB	2.66	0.42
1:A:580:VAL:HG11	1:A:623:ILE:HD11	2.02	0.42
1:A:605:GLU:HG3	1:A:608:GLN:HE21	1.85	0.42
1:A:613:VAL:C	1:A:615:ASP:N	2.71	0.42
1:B:378:LYS:HD2	1:B:378:LYS:HA	1.74	0.42
1:A:209:ARG:HA	1:A:212:PHE:HB3	2.02	0.42
1:A:619:PHE:C	1:A:619:PHE:CD1	2.93	0.42
1:B:764:ASP:O	1:B:768:VAL:HG13	2.19	0.42
1:A:374:TYR:O	1:A:379:ASP:HA	2.20	0.42
1:B:294:MET:CB	1:B:294:MET:SD	2.99	0.42
1:B:298:LEU:HD22	1:B:300:THR:HG21	2.02	0.42
1:B:786:ILE:HG12	1:B:833:ILE:HG23	2.02	0.42
1:B:782:ILE:HG23	1:B:806:LEU:HB3	2.01	0.42
1:B:296:GLU:OE1	1:B:296:GLU:CG	2.68	0.42
1:A:385:GLU:HB3	1:A:386:TYR:H	1.53	0.41
1:A:478:TYR:CE2	1:A:482:LEU:HD11	2.55	0.41
1:B:211:LYS:HG2	1:B:501:MET:CE	2.50	0.41
1:B:674:LEU:HB2	1:B:675:VAL:H	1.58	0.41
1:A:620:LEU:HA	1:A:623:ILE:HG22	2.02	0.41
1:A:771:ILE:HD13	1:A:774:LEU:HD12	2.01	0.41
1:B:300:THR:HA	1:B:303:ASN:HB2	2.02	0.41
1:A:491:ALA:O	1:A:495:THR:CG2	2.63	0.41
1:B:662:SER:HB2	1:B:717:LEU:HD21	2.02	0.41
1:B:768:VAL:HG23	1:B:769:LYS:N	2.36	0.41
1:A:454:TYR:HA	1:A:456:ARG:HD3	2.03	0.41
1:A:672:GLN:HA	1:A:672:GLN:NE2	2.35	0.41
1:A:787:HIS:O	1:A:789:LEU:HD22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:PRO:HB2	1:A:826:ARG:H	1.74	0.41
1:A:389:LYS:HA	1:A:389:LYS:HD2	1.82	0.41
1:A:593:ILE:HB	1:A:594:GLY:H	1.55	0.41
1:A:728:PHE:O	1:A:729:ASN:CB	2.69	0.41
1:A:771:ILE:N	1:A:772:PRO:HD2	2.36	0.41
1:B:209:ARG:HH22	1:B:549:ASP:CG	2.24	0.41
1:B:263:MET:HG2	1:B:273:VAL:CG1	2.50	0.41
1:B:718:LEU:HA	1:B:718:LEU:HD12	1.98	0.41
1:A:313:LEU:HB3	1:A:321:LYS:NZ	2.36	0.41
1:B:639:ASP:N	1:B:639:ASP:OD1	2.53	0.41
1:B:814:MET:O	1:B:816:TYR:O	2.39	0.41
1:B:436:LEU:HD21	1:B:481:THR:HB	2.03	0.41
1:B:672:GLN:CB	1:B:673:PRO:CD	2.80	0.41
1:A:652:ILE:HA	1:A:655:THR:HG23	2.03	0.40
1:B:268:ILE:O	1:B:268:ILE:HG23	2.20	0.40
1:B:785:MET:HA	1:B:785:MET:HE3	2.02	0.40
1:B:452:PRO:O	1:B:454:TYR:N	2.55	0.40
1:B:782:ILE:HD13	1:B:810:ALA:HB2	2.02	0.40
1:A:612:HIS:HA	1:B:231:ASN:ND2	2.37	0.40
1:B:428:VAL:CG1	1:B:429:THR:N	2.70	0.40
1:A:620:LEU:CA	1:A:623:ILE:HG22	2.52	0.40
1:A:425:ILE:HG21	1:A:428:VAL:CG2	2.52	0.40
1:A:533:ARG:HH11	1:A:533:ARG:HB2	1.87	0.40
1:A:574:GLU:OE1	1:A:577:ARG:NH1	2.54	0.40
1:B:346:ILE:HD12	1:B:347:LYS:N	2.33	0.40
1:B:641:ILE:O	1:B:645:GLN:CG	2.60	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	606/651 (93%)	503 (83%)	56 (9%)	47 (8%)	1 1
1	B	603/651 (93%)	486 (81%)	68 (11%)	49 (8%)	1 1
All	All	1209/1302 (93%)	989 (82%)	124 (10%)	96 (8%)	1 1

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ARG
1	A	317	ASP
1	A	421	SER
1	A	598	ALA
1	A	614	ARG
1	A	616	GLU
1	A	638	TYR
1	A	667	ALA
1	A	672	GLN
1	A	673	PRO
1	A	729	ASN
1	A	776	ILE
1	A	825	PRO
1	B	207	ILE
1	B	295	ASN
1	B	363	VAL
1	B	373	ALA
1	B	375	ALA
1	B	426	PRO
1	B	431	SER
1	B	446	LYS
1	B	451	ASP
1	B	453	VAL
1	B	454	TYR
1	B	457	TYR
1	B	458	SER
1	B	459	LEU
1	B	506	LEU
1	B	641	ILE
1	B	672	GLN
1	B	680	ASN
1	B	681	SER
1	B	764	ASP
1	A	252	GLN
1	A	293	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	361	LYS
1	A	373	ALA
1	A	385	GLU
1	A	387	SER
1	A	593	ILE
1	A	597	GLY
1	A	620	LEU
1	A	668	SER
1	A	670	LEU
1	A	671	ASP
1	A	679	ASP
1	A	728	PHE
1	A	757	ALA
1	A	760	PHE
1	A	768	VAL
1	A	780	SER
1	A	821	GLN
1	B	298	LEU
1	B	306	LYS
1	B	419	ASP
1	B	586	PHE
1	B	651	ASP
1	B	673	PRO
1	B	759	ASP
1	A	268	ILE
1	A	379	ASP
1	A	422	ARG
1	B	301	ASN
1	B	312	LYS
1	B	616	GLU
1	B	622	THR
1	B	636	ARG
1	B	678	ASP
1	B	826	ARG
1	A	294	MET
1	A	312	LYS
1	A	451	ASP
1	B	294	MET
1	B	318	LYS
1	B	379	ASP
1	B	382	LEU
1	B	384	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	422	ARG
1	B	428	VAL
1	B	630	ARG
1	B	827	GLU
1	A	232	PHE
1	A	363	VAL
1	A	567	THR
1	A	829	TYR
1	B	343	ALA
1	B	372	LYS
1	B	429	THR
1	A	381	GLY
1	A	594	GLY
1	A	772	PRO
1	B	376	SER
1	B	381	GLY
1	B	647	ALA
1	A	270	ILE
1	A	788	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	552/590 (94%)	465 (84%)	87 (16%)	2 4
1	B	549/590 (93%)	455 (83%)	94 (17%)	2 3
All	All	1101/1180 (93%)	920 (84%)	181 (16%)	2 3

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	GLU
1	A	206	ASN
1	A	207	ILE
1	A	208	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	209	ARG
1	A	231	ASN
1	A	246	ASN
1	A	248	THR
1	A	261	GLU
1	A	269	ASN
1	A	272	GLU
1	A	281	GLN
1	A	283	LEU
1	A	286	THR
1	A	294	MET
1	A	298	LEU
1	A	304	LYS
1	A	318	LYS
1	A	326	THR
1	A	333	ILE
1	A	347	LYS
1	A	361	LYS
1	A	362	LYS
1	A	369	THR
1	A	378	LYS
1	A	382	LEU
1	A	389	LYS
1	A	390	LEU
1	A	415	ILE
1	A	430	LEU
1	A	432	ILE
1	A	436	LEU
1	A	446	LYS
1	A	456	ARG
1	A	459	LEU
1	A	473	ARG
1	A	479	LEU
1	A	480	GLN
1	A	492	ILE
1	A	495	THR
1	A	506	LEU
1	A	513	LEU
1	A	515	LEU
1	A	529	LYS
1	A	532	ILE
1	A	533	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	542	THR
1	A	546	ARG
1	A	558	VAL
1	A	562	LEU
1	A	579	LEU
1	A	592	LYS
1	A	595	ARG
1	A	600	ILE
1	A	620	LEU
1	A	622	THR
1	A	623	ILE
1	A	633	GLU
1	A	642	LEU
1	A	655	THR
1	A	661	LEU
1	A	664	THR
1	A	670	LEU
1	A	672	GLN
1	A	683	THR
1	A	684	ASN
1	A	686	VAL
1	A	688	LEU
1	A	691	ARG
1	A	699	ASN
1	A	723	ILE
1	A	726	LEU
1	A	735	THR
1	A	744	LEU
1	A	751	LEU
1	A	754	ARG
1	A	773	ASN
1	A	776	ILE
1	A	779	LEU
1	A	782	ILE
1	A	785	MET
1	A	788	ILE
1	A	806	LEU
1	A	807	LYS
1	A	820	ILE
1	A	827	GLU
1	A	829	TYR
1	B	209	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	210	GLU
1	B	241	ILE
1	B	244	SER
1	B	261	GLU
1	B	271	VAL
1	B	281	GLN
1	B	283	LEU
1	B	286	THR
1	B	287	ASP
1	B	289	LEU
1	B	291	LYS
1	B	292	LYS
1	B	302	VAL
1	B	305	ILE
1	B	312	LYS
1	B	323	SER
1	B	336	LEU
1	B	361	LYS
1	B	362	LYS
1	B	363	VAL
1	B	364	GLU
1	B	365	GLN
1	B	371	PHE
1	B	372	LYS
1	B	378	LYS
1	B	385	GLU
1	B	389	LYS
1	B	395	ASN
1	B	396	GLN
1	B	423	LYS
1	B	430	LEU
1	B	442	LEU
1	B	446	LYS
1	B	454	TYR
1	B	457	TYR
1	B	459	LEU
1	B	461	ASP
1	B	479	LEU
1	B	481	THR
1	B	484	LEU
1	B	529	LYS
1	B	530	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	533	ARG
1	B	537	ILE
1	B	542	THR
1	B	543	LYS
1	B	551	ARG
1	B	559	LEU
1	B	567	THR
1	B	568	ASP
1	B	579	LEU
1	B	583	THR
1	B	593	ILE
1	B	603	VAL
1	B	620	LEU
1	B	623	ILE
1	B	624	THR
1	B	639	ASP
1	B	643	LEU
1	B	646	LEU
1	B	649	GLU
1	B	654	ILE
1	B	655	THR
1	B	659	SER
1	B	661	LEU
1	B	670	LEU
1	B	672	GLN
1	B	674	LEU
1	B	681	SER
1	B	684	ASN
1	B	709	LYS
1	B	710	ASN
1	B	717	LEU
1	B	718	LEU
1	B	733	GLN
1	B	734	GLU
1	B	744	LEU
1	B	754	ARG
1	B	761	SER
1	B	766	ASN
1	B	767	ILE
1	B	776	ILE
1	B	785	MET
1	B	789	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	799	LYS
1	B	803	ILE
1	B	804	ASP
1	B	806	LEU
1	B	812	GLN
1	B	820	ILE
1	B	822	TYR
1	B	827	GLU
1	B	832	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	231	ASN
1	A	236	ASN
1	A	250	ASN
1	A	269	ASN
1	A	276	GLN
1	A	280	GLN
1	A	293	ASN
1	A	303	ASN
1	A	324	ASN
1	A	356	ASN
1	A	396	GLN
1	A	439	HIS
1	A	480	GLN
1	A	536	ASN
1	A	563	ASN
1	A	573	HIS
1	A	626	GLN
1	A	672	GLN
1	A	699	ASN
1	A	733	GLN
1	A	766	ASN
1	A	787	HIS
1	A	790	ASN
1	A	808	ASN
1	A	812	GLN
1	A	821	GLN
1	B	214	ASN
1	B	221	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	250	ASN
1	B	281	GLN
1	B	380	HIS
1	B	396	GLN
1	B	397	HIS
1	B	536	ASN
1	B	645	GLN
1	B	719	ASN
1	B	731	GLN
1	B	766	ASN
1	B	770	ASN
1	B	812	GLN

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 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	612/651 (94%)	-0.01	31 (5%)	28	22	36, 49, 68, 80	0
1	B	609/651 (93%)	-0.02	21 (3%)	45	38	38, 49, 66, 76	0
All	All	1221/1302 (93%)	-0.02	52 (4%)	35	28	36, 49, 67, 80	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	831	THR	9.4
1	B	448	ALA	6.0
1	A	384	VAL	5.8
1	A	676	GLY	5.6
1	A	674	LEU	5.5
1	A	452	PRO	5.3
1	A	382	LEU	4.7
1	A	675	VAL	4.5
1	B	382	LEU	4.4
1	B	299	ALA	4.3
1	A	451	ASP	4.1
1	A	790	ASN	3.9
1	B	674	LEU	3.9
1	B	363	VAL	3.5
1	B	380	HIS	3.5
1	A	313	LEU	3.5
1	A	386	TYR	3.4
1	B	384	VAL	3.3
1	A	677	PRO	3.3
1	B	516	PHE	3.2
1	A	362	LYS	3.2
1	B	297	GLY	3.2
1	B	451	ASP	3.2
1	B	449	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	450	ASN	3.0
1	A	448	ALA	2.9
1	A	517	LYS	2.9
1	A	597	GLY	2.9
1	A	786	ILE	2.9
1	B	673	PRO	2.8
1	A	311	THR	2.8
1	A	728	PHE	2.8
1	A	293	ASN	2.8
1	B	530	ARG	2.7
1	B	446	LYS	2.7
1	B	379	ASP	2.6
1	A	822	TYR	2.6
1	A	381	GLY	2.5
1	A	598	ALA	2.5
1	B	358	ALA	2.5
1	A	817	ALA	2.4
1	A	833	ILE	2.4
1	B	529	LYS	2.4
1	B	675	VAL	2.3
1	A	730	LYS	2.3
1	B	317	ASP	2.2
1	A	380	HIS	2.2
1	A	205	ASN	2.1
1	A	449	GLU	2.1
1	A	827	GLU	2.0
1	B	454	TYR	2.0
1	A	789	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.