



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:31 PM UTC

PDB ID : 2RFO / pdb_00002rfo
Title : Crystal 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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

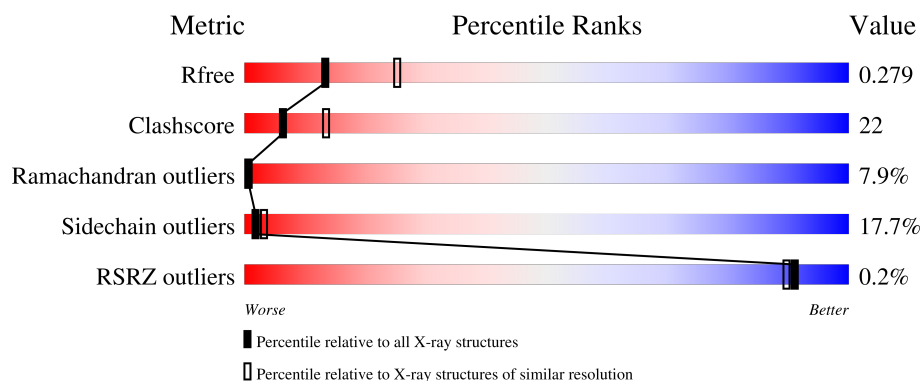
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	651	
1	B	651	

2 Entry composition

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			

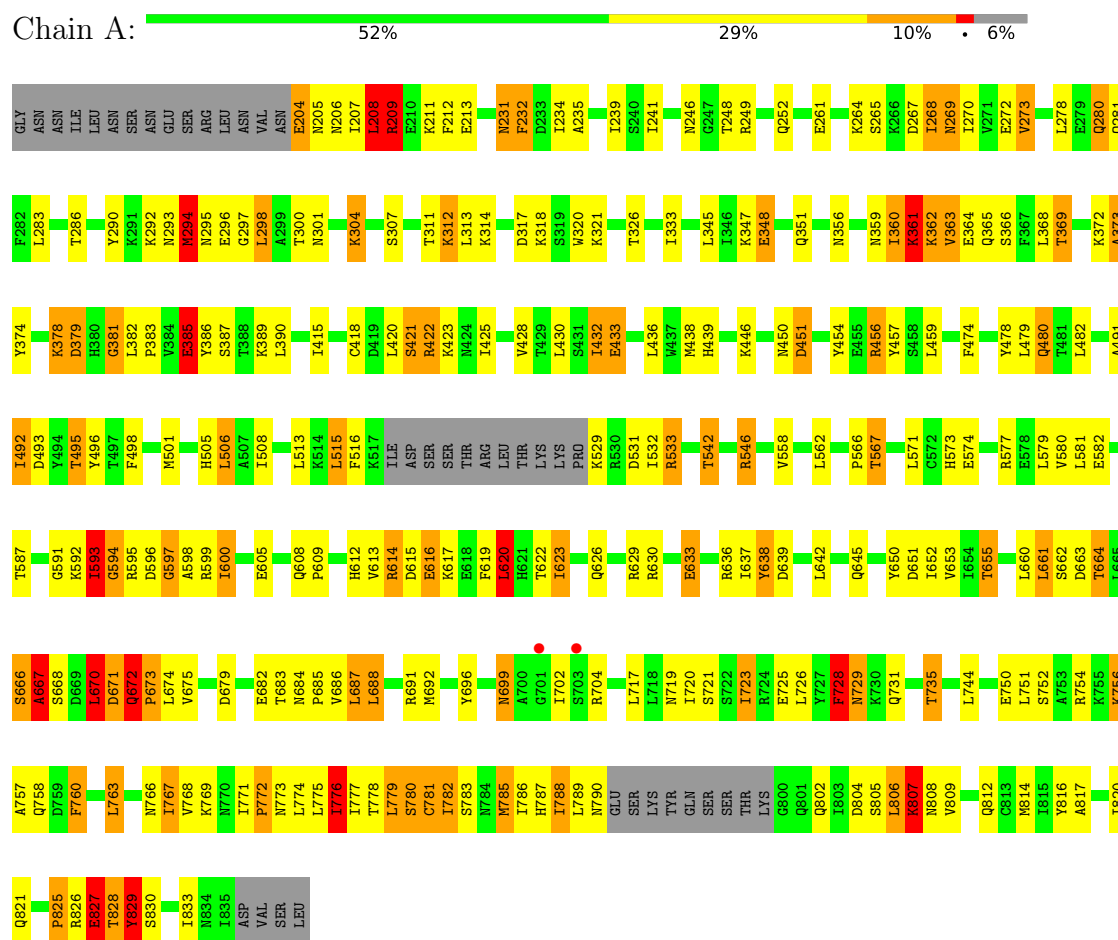
- Molecule 2 is water.

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

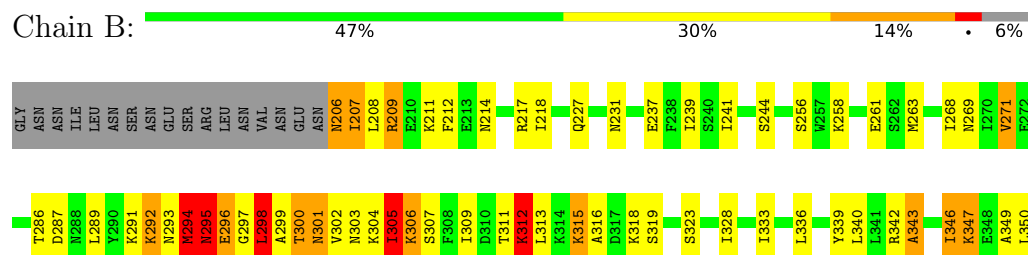
3 Residue-property plots

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: Nucleoporin NIC96



• Molecule 1: Nucleoporin NIC96



N790	G694	K617	P80	I443	V363	E364
GLU	L687	E618	K529	K446	Q365	S366
SER	L688	F619	R530	D447	F367	L368
LYS		L620	D531			
TYR		H621	I532			
GLN	R691	T622	R533	N450	D451	A372
SER	M692	I623	R533	D450	P452	A373
SER	Y696	T624	N536	D451	V453	Y374
K799			I537	Y454	P452	A375
G800	N699	A628	L538	E455	V453	S376
Q801		R629	T542	R456	S377	K378
Q802	K709	A631			Y457	D379
I803	N710	D632	B546		S458	H380
D804		E633			R459	G381
S805	L717	D634	D549		E460	L382
L806	L718	G635	P550		D461	P383
K807		R636	R551		F462	V384
	S721	I637			Q463	E385
A810	S722	Y638	L559			Y386
R811	I723	D639			F474	
Q812		S640	T567		S475	
C813	Q731	I641	D568		N476	
M814	W732	L642			Y477	
I815	Q733	L643	E574		L478	
Y816	E734	Y644			L479	
A817		Q645	B577		Q480	
	W739	L646	E578		T481	
I820		A647	L579		L482	
Q821	L742	E648			L483	
Y822	L743	E649	E582		L484	
R823	L744	E650	T583		L487	
M824	L745	D651	K584			D403
P825		I652	E585			
R826	R754	V653	F586		I492	R408
E827	K755	I654	T587		D493	
		T655				
	D759	S659	L590	Y496	C418	R417
Y829	F760	S659	G591		D419	
S830	S761	L660	K592		L420	
T831	W762	L661	I593	M501	S421	
L832	L763	S662	G594	D502	R422	
I833	D764		R595	A503	K423	
ASN			D596	H505	M424	
ILE	D765	L665	D596	H505	I425	
ASP	N766	S666	G597	L506	R426	
VAL	I767		A598		P426	
SER	W768	D669	R599	L510	A427	
LEU	K769	L670	I600		V428	
	N770	D671		F516	L429	
	I771		V603	LYS	T430	
	P772	Q672		ILE	S431	
	I776	L674	R607	ASP	I432	
		V675	Q608	SER	E433	
		P673	P609	SER	D434	
	I782	P677	L610	THR	W435	
		L611		ARG	L436	
	W785	D678	L611	LEU	W437	
	I786	D679	R614	THR	W438	
		N680	D515	LYS		
	L789	S681	E616	LYS	L442	

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.94%)	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)	0.29 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.82	9/5048 (0.2%)	1.06	17/6825 (0.2%)
1	B	1.19	35/5022 (0.7%)	1.16	32/6790 (0.5%)
All	All	1.02	44/10070 (0.4%)	1.11	49/13615 (0.4%)

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 (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	GLU	CD-OE1	30.95	1.84	1.25
1	B	597	GLY	CA-C	23.51	2.07	1.52
1	B	636	ARG	CZ-NH1	16.21	1.55	1.32
1	B	790	ASN	CG-OD1	16.06	1.54	1.23
1	B	295	ASN	CG-OD1	15.35	1.52	1.23
1	B	296	GLU	CD-OE2	-15.32	0.96	1.25
1	B	597	GLY	N-CA	12.37	1.62	1.44
1	B	294	MET	SD-CE	12.16	2.10	1.79
1	B	296	GLU	CG-CD	11.50	1.80	1.52
1	A	297	GLY	C-O	11.44	1.34	1.23
1	B	294	MET	CG-SD	9.96	2.05	1.80
1	B	678	ASP	CG-OD2	9.39	1.43	1.25
1	A	667	ALA	N-CA	8.85	1.57	1.46
1	A	667	ALA	CA-CB	8.67	1.68	1.53
1	B	594	GLY	C-N	8.66	1.45	1.33
1	B	789	LEU	CG-CD1	7.69	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	ASN	CG-ND2	7.62	1.49	1.33
1	B	296	GLU	CB-CG	7.46	1.74	1.52
1	B	678	ASP	CG-OD1	7.43	1.39	1.25
1	A	666	SER	C-N	7.28	1.43	1.33
1	B	504	VAL	CA-CB	6.91	1.62	1.54
1	B	298	LEU	C-N	6.74	1.43	1.33
1	A	667	ALA	C-O	6.41	1.32	1.24
1	B	593	ILE	CA-CB	6.38	1.61	1.53
1	B	636	ARG	CD-NE	6.24	1.54	1.46
1	B	790	ASN	CG-ND2	6.23	1.46	1.33
1	B	600	ILE	N-CA	6.14	1.51	1.46
1	A	296	GLU	C-O	6.13	1.31	1.24
1	A	666	SER	C-O	6.04	1.31	1.24
1	B	419	ASP	CG-OD1	6.02	1.36	1.25
1	B	300	THR	CB-OG1	5.97	1.53	1.43
1	A	667	ALA	C-N	5.87	1.42	1.33
1	B	419	ASP	CG-OD2	5.74	1.36	1.25
1	B	294	MET	C-O	5.73	1.31	1.24
1	A	296	GLU	C-N	5.71	1.39	1.33
1	B	298	LEU	C-O	5.66	1.31	1.24
1	B	596	ASP	C-O	5.62	1.30	1.24
1	B	530	ARG	NE-CZ	5.59	1.39	1.33
1	B	592	LYS	CA-C	5.55	1.59	1.52
1	B	628	ALA	C-O	5.52	1.30	1.24
1	B	593	ILE	CB-CG1	5.37	1.64	1.53
1	B	599	ARG	CA-CB	5.31	1.59	1.52
1	B	598	ALA	C-O	5.23	1.30	1.23
1	B	392	THR	CB-OG1	5.05	1.51	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	597	GLY	N-CA-C	-13.96	93.12	116.01
1	B	296	GLU	CG-CD-OE2	11.46	144.77	118.40
1	B	296	GLU	CG-CD-OE1	-10.24	94.85	118.40
1	B	458	SER	N-CA-C	8.48	128.87	110.80
1	B	639	ASP	N-CA-C	-8.48	97.73	110.28
1	B	769	LYS	N-CA-C	-7.99	100.28	110.19
1	B	597	GLY	O-C-N	7.90	130.73	122.51
1	A	672	GLN	CA-C-N	7.71	129.48	119.84
1	A	672	GLN	C-N-CA	7.71	129.48	119.84
1	B	305	ILE	N-CA-C	-7.67	99.60	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ASN	OD1-CG-ND2	7.48	130.08	122.60
1	B	592	LYS	CA-C-N	-7.05	113.70	122.93
1	B	592	LYS	C-N-CA	-7.05	113.70	122.93
1	A	295	ASN	N-CA-C	7.04	120.70	110.28
1	B	430	LEU	N-CA-C	-6.95	99.67	110.17
1	B	425	ILE	CA-C-N	6.95	128.53	119.84
1	B	425	ILE	C-N-CA	6.95	128.53	119.84
1	B	790	ASN	OD1-CG-ND2	6.77	129.37	122.60
1	B	296	GLU	CB-CG-CD	-6.56	101.45	112.60
1	B	805	SER	N-CA-C	-6.37	104.41	111.36
1	B	457	TYR	N-CA-C	6.25	124.12	110.80
1	B	829	TYR	N-CA-C	6.20	119.64	109.85
1	B	505	HIS	N-CA-C	-6.14	101.20	110.28
1	A	206	ASN	N-CA-C	-6.06	104.79	111.82
1	B	672	GLN	N-CA-C	5.98	123.02	109.81
1	A	807	LYS	N-CA-C	-5.93	105.29	113.18
1	A	828	THR	N-CA-C	-5.87	106.75	112.97
1	B	801	GLN	N-CA-C	-5.67	106.32	113.18
1	A	418	CYS	N-CA-C	5.63	119.32	112.23
1	A	777	ILE	N-CA-C	-5.59	104.47	112.35
1	B	816	TYR	N-CA-C	-5.47	103.27	110.33
1	A	593	ILE	N-CA-C	5.38	120.53	109.34
1	B	271	VAL	N-CA-C	5.35	116.13	110.72
1	A	241	ILE	CB-CA-C	-5.31	105.17	111.97
1	A	758	GLN	N-CA-C	-5.25	104.81	111.11
1	A	365	GLN	N-CA-C	-5.23	106.73	113.01
1	A	781	CYS	N-CA-C	-5.21	105.49	111.07
1	B	611	LEU	N-CA-C	-5.20	102.36	110.42
1	A	600	ILE	CB-CA-C	5.17	117.14	111.04
1	B	676	GLY	CA-C-N	5.16	126.29	119.84
1	B	676	GLY	C-N-CA	5.16	126.29	119.84
1	A	506	LEU	N-CA-C	-5.11	105.60	111.07
1	B	421	SER	N-CA-C	-5.10	103.80	110.53
1	A	827	GLU	N-CA-C	5.10	117.92	107.37
1	B	478	TYR	N-CA-C	5.10	117.22	111.11
1	B	621	HIS	N-CA-C	-5.09	103.43	110.35
1	A	208	LEU	CA-CB-CG	5.07	134.06	116.30
1	B	592	LYS	CA-C-O	-5.04	114.56	120.60
1	B	679	ASP	N-CA-C	5.03	118.31	110.32

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

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	203	0
1	B	4935	0	4989	241	0
2	A	37	0	0	0	0
2	B	51	0	0	4	0
All	All	9984	0	10000	439	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 22.

All (439) 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:CG	1:B:296:GLU:CB	1.74	1.61
1:B:789:LEU:CG	1:B:789:LEU:CD1	1.77	1.61
1:B:296:GLU:CG	1:B:296:GLU:CD	1.80	1.52
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:C	1:B:597:GLY:CA	2.07	1.26
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	1.20
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ASP:O	1:A:664:THR:HG23	1.56	1.05
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.25	1.00
1:B:755:LYS:O	1:B:759:ASP:HB2	1.62	0.99
1:A:480:GLN:H	1:A:480:GLN:HE21	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:269:ASN:C	1:A:269:ASN:HD22	1.84	0.85
1:A:362:LYS:HE3	1:A:362:LYS:HA	1.57	0.84
1:B:595:ARG:HA	1:B:691:ARG:HH12	1.42	0.84
1:B:769:LYS:HZ2	1:B:770:ASN:H	1.24	0.83
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:HA	1:B:812:GLN:HE21	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:218:ILE:HD12	1:B:237:GLU:HG2	1.62	0.80
1:A:699:ASN:C	1:A:699:ASN:HD22	1.90	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:769:LYS:HZ2	1:B:770:ASN:N	1.82	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: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:HA	1:A:378:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PHE:N	1:B:501:MET:HE1	2.03	0.73
1:A:209:ARG:HH11	1:A:209:ARG:CG	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:B:692:MET:HE3	1:B:696:TYR:CE1	2.25	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: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:B:739:MET:HE1	1:B:745:LEU:HD22	1.74	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:A:211:LYS:C	1:A:501:MET:HE1	2.18	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
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:A:814:MET:HE2	1:A:814:MET:HA	1.76	0.67
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:CD1	1:B:789:LEU:CD2	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:502:ASP:O	1:B:505:HIS:O	2.15	0.65
1:A:767:ILE:C	1:A:769:LYS:H	2.04	0.65
1:A:267:ASP:HB3	1:B:614:ARG:HH21	1.61	0.65
1:B:364:GLU:C	1:B:366:SER:H	2.03	0.64
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:HE21	1:B:812:GLN:CA	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:B:211:LYS:C	1:B:501:MET:HE1	2.22	0.63
1:A:660:LEU:O	1:A:664:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:SER:HA	2:B:874:HOH:O	2.00	0.62
1:A:672:GLN:HA	1:A:672:GLN:HE21	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: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:209:ARG:HG3	1:A:209:ARG:NH1	2.04	0.61
1:A:421:SER:O	1:A:422:ARG:C	2.43	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
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:B:293:ASN:C	1:B:295:ASN:H	2.08	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:A:378:LYS:HA	1:A:378:LYS:HZ3	1.67	0.59
1:B:296:GLU:CB	1:B:296:GLU:CD	2.75	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:313:LEU:HB3	1:A:321:LYS:HZ2	1.66	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:B:531:ASP:CG	1:B:536:ASN:HD22	2.10	0.59
1:A:614:ARG:O	1:A:614:ARG:HG2	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:HD13	1:B:674:LEU:N	2.18	0.59
1:A:670:LEU:O	1:A:671:ASP:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:613:VAL:C	1:A:615:ASP:H	2.11	0.57
1:A:771:ILE:O	1:A:772:PRO:C	2.46	0.57
1:A:211:LYS:HG2	1:A:501:MET:HE1	1.85	0.57
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:362:LYS:C	1:B:364:GLU:H	2.13	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
1:B:403:ASP:OD2	1:B:403:ASP:N	2.34	0.56
1:B:212:PHE:HA	1:B:501:MET:HE1	1.88	0.56
1:A:208:LEU:O	1:A:209:ARG:HB2	2.04	0.56
1:A:211:LYS:O	1:A:501:MET:HE1	2.06	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: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:B:669:ASP:CG	1:B:670:LEU:H	2.13	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:211:LYS:HG2	1:A:501:MET:CE	2.37	0.55
1:A:439:HIS:HD2	1:A:457:TYR:OH	1.89	0.55
1:A:782:ILE:O	1:A:786:ILE:HG12	2.05	0.55
1:B:212:PHE:CA	1:B:501:MET:HE1	2.36	0.55
1:B:425:ILE:HD12	1:B:438:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:290:TYR:C	1:A:292:LYS:H	2.13	0.54
1:B:372:LYS:O	1:B:373:ALA:CB	2.55	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:632:ASP:C	1:B:634:ASP:H	2.15	0.54
1:B:802:GLN:O	1:B:805:SER:HB3	2.07	0.54
1:A:782:ILE:HD11	1:A:809:VAL:HB	1.90	0.53
1:A:828:THR:C	1:A:830:SER:H	2.14	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:425:ILE:HD13	1:A:438:MET:HE3	1.90	0.53
1:B:463:GLN:HB3	1:B:487:LEU:HD21	1.91	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
1:A:617:LYS:N	1:A:617:LYS:HD2	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: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:B:211:LYS:HG2	1:B:501:MET:HE2	1.92	0.52
1:A:781:CYS:C	1:A:783:SER:H	2.17	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:B:829:TYR:C	1:B:830:SER:HG	2.18	0.52
1:A:420:LEU:C	1:A:421:SER:O	2.51	0.51
1:B:207:ILE:HG13	1:B:208:LEU:N	2.25	0.51
1:A:779:LEU:O	1:A:780:SER:HB2	2.09	0.51
1:A:790:ASN:HD22	1:A:790:ASN:H	1.57	0.51
1:B:375:ALA:C	1:B:377:SER:H	2.19	0.51
1:B:692:MET:HE2	1:B:696:TYR:HE1	1.74	0.51
1:B:418:CYS:O	1:B:419:ASP:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:339:TYR:O	1:B:342:ARG:O	2.28	0.51
1:B:785:MET:HE3	1:B:785:MET:HA	1.92	0.51
1:B:635:GLY:O	1:B:637:ILE:HG13	2.11	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:B:362:LYS:O	1:B:364:GLU:N	2.44	0.51
1:B:516:PHE:HD2	1:B:516:PHE:O	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:A:592:LYS:HG3	1:A:593:ILE:N	2.26	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:B:665:LEU:HD21	1:B:721:SER:HB3	1.94	0.50
1:A:616:GLU:N	1:A:616:GLU:OE1	2.45	0.49
1:B:760:PHE:C	1:B:762:ASN:H	2.19	0.49
1:B:674:LEU:HA	1:B:677:PRO:HB2	1.94	0.49
1:B:353:LEU:HB3	1:B:368:LEU:HD23	1.95	0.49
1:A:231:ASN:O	1:A:232:PHE:C	2.54	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:HE3	1:A:617:LYS:HA	1.95	0.49
1:B:477:TYR:O	1:B:481:THR:HG22	2.12	0.49
1:A:779:LEU:HD21	1:A:814:MET:HE3	1.95	0.49
1:B:597:GLY:C	1:B:597:GLY:N	2.70	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:364:GLU:C	1:B:366:SER:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:HG3	1:A:313:LEU:N	2.27	0.48
1:A:596:ASP:O	1:A:597:GLY:C	2.56	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:298:LEU:C	1:B:300:THR:HG23	2.38	0.48
1:B:630:ARG:O	1:B:636:ARG:NH2	2.47	0.48
1:A:663:ASP:C	1:A:664:THR:CG2	2.87	0.48
1:B:361:LYS:HE3	1:B:362:LYS:HE2	1.95	0.48
1:B:812:GLN:HA	1:B:812:GLN:NE2	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: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:A:699:ASN:C	1:A:699:ASN:ND2	2.62	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: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:432:ILE:HD11	1:A:474:PHE:HD2	1.80	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
1:A:637:ILE:O	1:A:638:TYR:CB	2.62	0.47
1:A:767:ILE:C	1:A:769:LYS:N	2.69	0.47
1:B:443:ILE:HG12	1:B:458:SER:HB3	1.97	0.47
1:B:456:ARG:HG3	1:B:457:TYR:H	1.80	0.47
1:B:763:LEU:O	1:B:763:LEU:HG	2.14	0.47
1:A:619:PHE:C	1:A:619:PHE:CD1	2.93	0.47
1:B:822:TYR:O	1:B:823:ARG:HB2	2.14	0.47
1:A:778:THR:HG22	1:A:782:ILE:HD12	1.96	0.47
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:CG2	1:B:820:ILE:O	2.63	0.46
1:A:613:VAL:C	1:A:615:ASP:N	2.71	0.46
1:A:782:ILE:O	1:A:782:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLN:HG2	1:B:785:MET:SD	2.55	0.46
1:B:396:GLN:HA	1:B:396:GLN:NE2	2.29	0.46
1:B:766:ASN:HD22	1:B:766:ASN:HA	1.58	0.46
1:A:531:ASP:OD1	1:A:533:ARG:NH1	2.49	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:209:ARG:HH22	1:B:549:ASP:CG	2.24	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:B:699:ASN:C	1:B:699:ASN:OD1	2.58	0.45
1:A:666:SER:O	1:A:667:ALA:HB2	2.15	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: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
1:B:350:LEU:HD21	1:B:372:LYS:HG2	1.99	0.44
1:A:492:ILE:HG13	1:A:493:ASP:N	2.32	0.44
1:A:615:ASP:C	1:A:617:LYS:N	2.75	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:A:828:THR:C	1:A:830:SER:N	2.76	0.44
1:A:605:GLU:O	1:A:608:GLN:HG3	2.17	0.44
1:A:614:ARG:HG3	1:A:614:ARG:HH11	1.82	0.44
1:A:779:LEU:HA	1:A:782:ILE:HG22	2.00	0.44
1:B:296:GLU:CG	1:B:296:GLU:CA	2.83	0.44
1:A:567:THR:O	1:A:571:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:231:ASN:ND2	1:A:231:ASN:N	2.61	0.44
1:A:581:LEU:O	1:A:582:GLU:CG	2.59	0.44
1:A:666:SER:HA	1:A:773:ASN:OD1	2.18	0.44
1:A:682:GLU:HA	1:A:688:LEU:HB2	2.00	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:B:804:ASP:OD1	1:B:804:ASP:C	2.61	0.44
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:HA	1:B:785:MET:CE	2.49	0.43
1:B:799:LYS:HD3	1:B:799:LYS:HA	1.59	0.43
1:A:756:LYS:O	1:A:816:TYR:CE1	2.71	0.43
1:A:775:LEU:C	1:A:776:ILE:HG23	2.44	0.43
1:B:542:THR:HG21	2:B:882:HOH:O	2.18	0.43
1:B:666:SER:CB	1:B:769:LYS:HG3	2.43	0.43
1:B:767:ILE:O	1:B:769:LYS:O	2.36	0.43
1:B:767:ILE:C	1:B:769:LYS:O	2.61	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:HD2	1:A:312:LYS:HA	1.89	0.43
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:269:ASN:C	1:A:269:ASN:ND2	2.58	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:A:829:TYR:CD1	1:A:829:TYR:C	2.96	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:585:GLU:C	1:B:586:PHE:O	2.58	0.43
1:B:293:ASN:C	1:B:295:ASN:N	2.75	0.42
1:B:516:PHE:O	1:B:516:PHE:CD2	2.72	0.42
1:A:265:SER:HB2	1:B:609:PRO:HA	2.01	0.42
1:A:650:TYR:CE1	1:A:702:ILE:HG12	2.54	0.42
1:A:670:LEU:O	1:A:670:LEU:HD12	2.19	0.42
1:B:629:ARG:C	1:B:631:ALA:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:TYR:C	1:A:292:LYS:N	2.78	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: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: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:SD	1:B:294:MET:CB	2.99	0.42
1:B:298:LEU:HD22	1:B:300:THR:HG21	2.02	0.42
1:B:362:LYS:C	1:B:364:GLU:N	2.78	0.42
1:B:782:ILE:HG23	1:B:806:LEU:HB3	2.01	0.42
1:B:786:ILE:HG12	1:B:833:ILE:HG23	2.02	0.42
1:B:822:TYR:C	1:B:824:MET:H	2.27	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:A:653:VAL:HG11	1:A:692:MET:HE2	2.01	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:B:632:ASP:C	1:B:634:ASP:N	2.78	0.41
1:A:491:ALA:O	1:A:495:THR:CG2	2.63	0.41
1:B:211:LYS:HG2	1:B:501:MET:CE	2.50	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
1:A:825:PRO:HB2	1:A:826:ARG:H	1.74	0.41
1:A:389:LYS:HD2	1:A:389:LYS:HA	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:263:MET:HG2	1:B:273:VAL:CG1	2.50	0.41
1:B:296:GLU:CG	1:B:296:GLU:OE1	2.68	0.41
1:B:718:LEU:HD12	1:B:718:LEU:HA	1.98	0.41
1:B:815:ILE:C	1:B:816:TYR:O	2.63	0.41
1:A:364:GLU:C	1:A:366:SER:N	2.79	0.41
1:B:436:LEU:HD21	1:B:481:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:ASP:OD1	1:B:639:ASP:N	2.53	0.41
1:B:814:MET:O	1:B:816:TYR:O	2.39	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:269:ASN:OD1	1:B:269:ASN:C	2.63	0.40
1:B:452:PRO:O	1:B:454:TYR:N	2.55	0.40
1:B:652:ILE:O	1:B:653:VAL:C	2.63	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:474:PHE:O	1:B:475:SER:C	2.61	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	0
All	All	1209/1302 (93%)	989 (82%)	124 (10%)	96 (8%)	1	0

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	457 (83%)	95 (17%)	2	3
1	B	549/590 (93%)	449 (82%)	100 (18%)	2	3
All	All	1101/1180 (93%)	906 (82%)	195 (18%)	2	3

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	GLU
1	A	207	ILE
1	A	208	LEU
1	A	209	ARG
1	A	231	ASN
1	A	234	ILE
1	A	246	ASN
1	A	248	THR
1	A	264	LYS
1	A	269	ASN
1	A	272	GLU
1	A	273	VAL

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Mol	Chain	Res	Type
1	A	280	GLN
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	348	GLU
1	A	351	GLN
1	A	360	ILE
1	A	361	LYS
1	A	362	LYS
1	A	368	LEU
1	A	369	THR
1	A	378	LYS
1	A	382	LEU
1	A	385	GLU
1	A	390	LEU
1	A	415	ILE
1	A	423	LYS
1	A	430	LEU
1	A	432	ILE
1	A	433	GLU
1	A	436	LEU
1	A	446	LYS
1	A	456	ARG
1	A	459	LEU
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
1	A	542	THR

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Mol	Chain	Res	Type
1	A	546	ARG
1	A	558	VAL
1	A	562	LEU
1	A	579	LEU
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	686	VAL
1	A	687	LEU
1	A	688	LEU
1	A	699	ASN
1	A	723	ILE
1	A	726	LEU
1	A	735	THR
1	A	744	LEU
1	A	750	GLU
1	A	751	LEU
1	A	754	ARG
1	A	756	LYS
1	A	763	LEU
1	A	767	ILE
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	A	833	ILE
1	B	209	ARG

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Mol	Chain	Res	Type
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	315	LYS
1	B	323	SER
1	B	336	LEU
1	B	346	ILE
1	B	347	LYS
1	B	361	LYS
1	B	362	LYS
1	B	363	VAL
1	B	364	GLU
1	B	365	GLN
1	B	372	LYS
1	B	378	LYS
1	B	385	GLU
1	B	395	ASN
1	B	396	GLN
1	B	398	ILE
1	B	423	LYS
1	B	430	LEU
1	B	433	GLU
1	B	442	LEU
1	B	446	LYS
1	B	457	TYR
1	B	459	LEU
1	B	479	LEU
1	B	481	THR
1	B	484	LEU
1	B	504	VAL
1	B	529	LYS

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Mol	Chain	Res	Type
1	B	530	ARG
1	B	533	ARG
1	B	537	ILE
1	B	538	LEU
1	B	542	THR
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	607	ARG
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	717	LEU
1	B	718	LEU
1	B	723	ILE
1	B	733	GLN
1	B	734	GLU
1	B	739	MET
1	B	742	LEU
1	B	744	LEU
1	B	754	ARG
1	B	761	SER
1	B	766	ASN

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Mol	Chain	Res	Type
1	B	767	ILE
1	B	769	LYS
1	B	776	ILE
1	B	785	MET
1	B	786	ILE
1	B	789	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) 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	295	ASN
1	A	303	ASN
1	A	324	ASN
1	A	356	ASN
1	A	396	GLN
1	A	439	HIS
1	A	450	ASN
1	A	480	GLN
1	A	536	ASN
1	A	563	ASN
1	A	573	HIS
1	A	626	GLN
1	A	645	GLN
1	A	658	ASN
1	A	672	GLN

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Mol	Chain	Res	Type
1	A	699	ASN
1	A	733	GLN
1	A	766	ASN
1	A	790	ASN
1	A	808	ASN
1	A	812	GLN
1	A	821	GLN
1	B	214	ASN
1	B	250	ASN
1	B	281	GLN
1	B	356	ASN
1	B	396	GLN
1	B	536	ASN
1	B	608	GLN
1	B	719	ASN
1	B	731	GLN
1	B	762	ASN
1	B	766	ASN
1	B	770	ASN
1	B	790	ASN

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 oligosaccharides 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 [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	612/651 (94%)	-1.15	2 (0%) 90 88	36, 49, 68, 80	0
1	B	609/651 (93%)	-1.30	0 100 100	38, 49, 66, 76	0
All	All	1221/1302 (93%)	-1.22	2 (0%) 91 90	36, 49, 67, 80	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	703	SER	2.8
1	A	701	GLY	2.6

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 oligosaccharides 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.