



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:36 AM GMT

PDB ID : 2P8Q  
Title : Crystal Structure of human Importin beta bound to the Snurportin1 IBB-domain  
Authors : Mitrousis, G.; Cingolani, G.  
Deposited on : 2007-03-22  
Resolution : 2.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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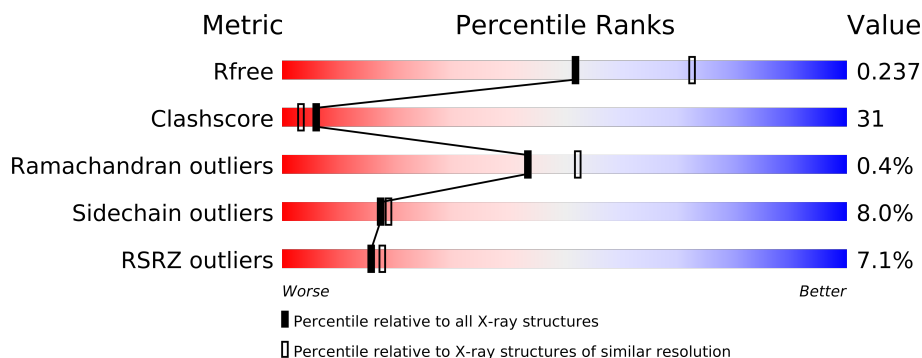
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	876	
2	B	40	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7471 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Importin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	873	Total	C	N	O	S	0	0	0
			6782	4273	1136	1326	47			

- Molecule 2 is a protein called Snurportin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	0	0	0
			344	210	73	61			

- Molecule 3 is water.

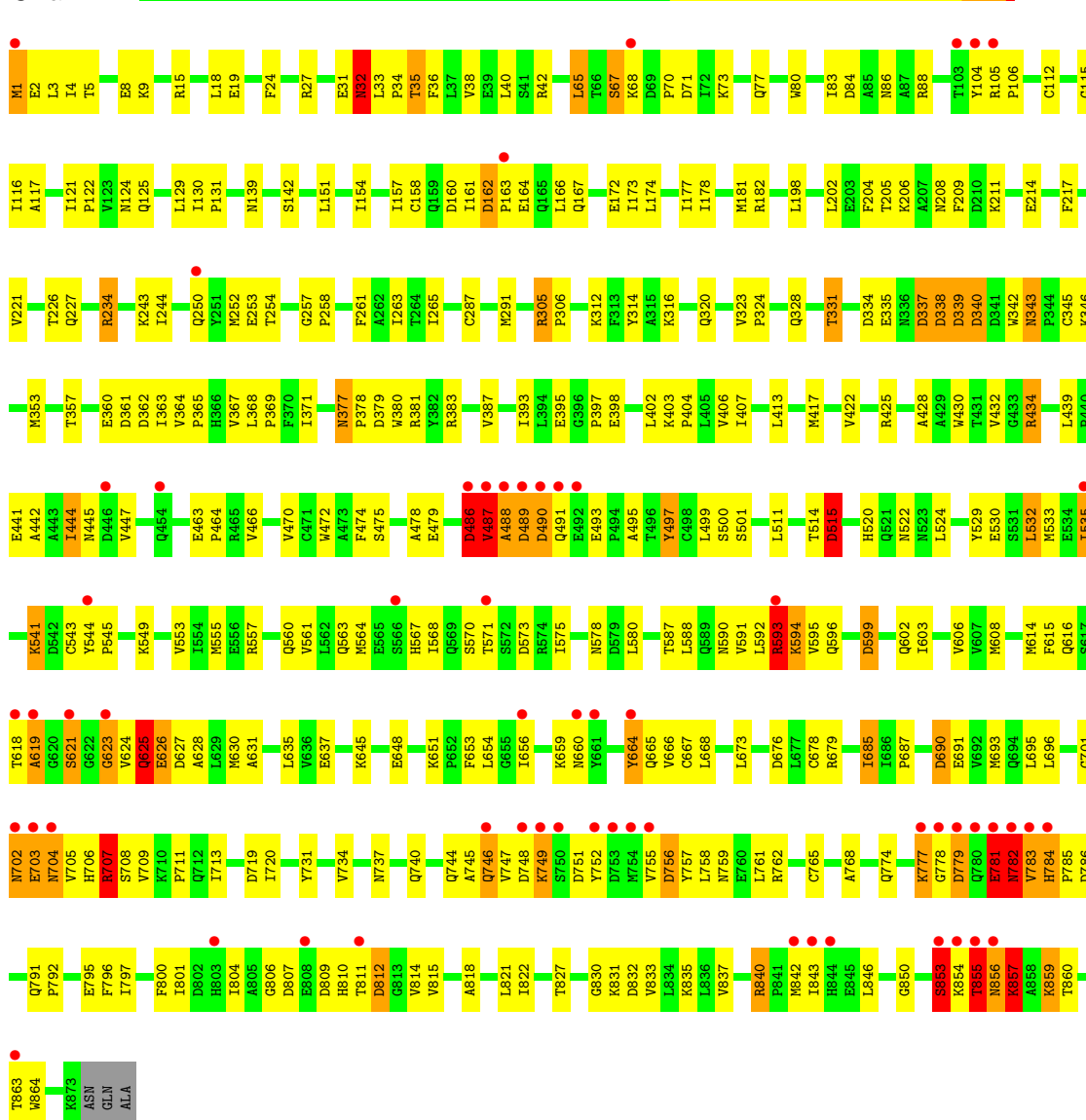
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	332	Total	O	0	0
			332	332		
3	B	13	Total	O	0	0
			13	13		

### 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: Importin beta-1 subunit

Chain A:



#### • Molecule 2: Snurportin-1

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.75Å 97.89Å 84.29Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35 39.04 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-2.35) 94.2 (39.04-2.31)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.250 0.236 , 0.237	Depositor DCC
$R_{free}$ test set	4282 reflections (10.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.0	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 43297 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7471	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.32	0/6893	0.56	18/9360 (0.2%)
2	B	0.25	0/348	0.42	0/458
All	All	0.32	0/7241	0.56	18/9818 (0.2%)

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	24
2	B	0	2
All	All	0	26

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	338	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	361	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	334	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	690	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	160	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	362	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	339	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	337	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	786	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	486	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	832	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	573	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	162	ASP	CB-CG-OD2	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	779	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	748	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	812	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	756	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	487	VAL	Peptide
1	A	488	ALA	Peptide
1	A	489	ASP	Peptide
1	A	490	ASP	Peptide
1	A	593	ARG	Peptide
1	A	619	ALA	Peptide
1	A	623	GLY	Peptide
1	A	625	GLN	Peptide
1	A	701	GLY	Peptide
1	A	702	ASN	Peptide
1	A	703	GLU	Peptide
1	A	704	ASN	Peptide
1	A	707	ARG	Peptide
1	A	749	LYS	Peptide
1	A	756	ASP	Peptide
1	A	777	LYS	Peptide
1	A	781	GLU	Peptide
1	A	782	ASN	Peptide
1	A	783	VAL	Peptide
1	A	784	HIS	Peptide
1	A	830	GLY	Peptide
1	A	853	SER	Peptide
1	A	855	THR	Peptide
1	A	857	LYS	Peptide
2	B	38	LEU	Peptide
2	B	40	GLN	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,



and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6782	0	6781	417	0
2	B	344	0	359	41	0
3	A	332	0	0	56	0
3	B	13	0	0	4	0
All	All	7471	0	7140	441	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (441) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:702:ASN:CB	1:A:703:GLU:HG3	1.47	1.41
1:A:702:ASN:HB3	1:A:703:GLU:CG	1.48	1.40
2:B:37:SER:C	2:B:38:LEU:HD13	1.48	1.31
1:A:316:LYS:HD2	3:A:1193:HOH:O	1.40	1.21
1:A:702:ASN:O	1:A:705:VAL:HG23	1.37	1.19
1:A:707:ARG:HD2	1:A:757:TYR:CD1	1.78	1.18
1:A:777:LYS:HG2	1:A:778:GLY:N	1.55	1.15
1:A:855:THR:HG22	1:A:856:ASN:N	1.57	1.14
1:A:397:PRO:HB2	1:A:402:LEU:HD11	1.29	1.14
1:A:593:ARG:HH11	1:A:593:ARG:HG3	1.11	1.13
1:A:777:LYS:HG2	1:A:778:GLY:H	1.06	1.12
1:A:68:LYS:HD2	1:A:68:LYS:H	1.16	1.10
1:A:105:ARG:HB3	1:A:106:PRO:CD	1.80	1.10
1:A:860:THR:O	1:A:863:THR:HG22	1.51	1.10
1:A:856:ASN:O	1:A:857:LYS:HG2	1.53	1.07
1:A:514:THR:HG21	1:A:557:ARG:HH12	1.19	1.05
2:B:38:LEU:HD13	2:B:38:LEU:N	1.66	1.05
1:A:105:ARG:HB3	1:A:106:PRO:HD3	1.36	1.04
1:A:708:SER:HB2	3:A:1203:HOH:O	1.56	1.03
1:A:320:GLN:HG3	3:A:879:HOH:O	1.57	1.03
1:A:619:ALA:HB2	1:A:623:GLY:HA3	1.42	1.02
1:A:488:ALA:HB1	1:A:489:ASP:HA	1.38	1.02
1:A:783:VAL:O	1:A:785:PRO:HD3	1.59	1.01
1:A:855:THR:CG2	1:A:856:ASN:H	1.73	1.01
1:A:783:VAL:C	1:A:785:PRO:HD3	1.79	1.01
1:A:342:TRP:NE1	2:B:26:PRO:HD2	1.76	1.00
1:A:619:ALA:HA	1:A:621:SER:H	1.27	0.99
1:A:511:LEU:O	1:A:514:THR:HG22	1.61	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:855:THR:HG22	1:A:856:ASN:H	0.86	0.99
1:A:702:ASN:HD22	1:A:703:GLU:HG2	1.24	0.99
1:A:478:ALA:HB1	1:A:535:ILE:HD13	1.42	0.99
1:A:593:ARG:CG	1:A:593:ARG:HH11	1.75	0.99
1:A:342:TRP:CD1	2:B:26:PRO:HD2	1.96	0.99
1:A:778:GLY:HA3	1:A:781:GLU:OE2	1.62	0.98
2:B:37:SER:C	2:B:38:LEU:CD1	2.30	0.98
1:A:856:ASN:C	1:A:857:LYS:HG2	1.79	0.98
1:A:707:ARG:CD	1:A:757:TYR:CD1	2.47	0.97
1:A:702:ASN:ND2	1:A:703:GLU:HG2	1.80	0.97
1:A:784:HIS:N	1:A:785:PRO:HD3	1.79	0.97
1:A:154:ILE:HG21	1:A:177:ILE:HD11	1.44	0.96
1:A:162:ASP:OD2	1:A:163:PRO:HD2	1.67	0.95
1:A:544:TYR:N	1:A:545:PRO:HD2	1.82	0.94
1:A:857:LYS:HB3	1:A:860:THR:OG1	1.66	0.94
1:A:124:ASN:HB3	3:A:1185:HOH:O	1.68	0.93
1:A:342:TRP:CD1	2:B:26:PRO:CD	2.53	0.92
1:A:707:ARG:HD3	1:A:757:TYR:CD2	2.06	0.90
1:A:807:ASP:HB3	1:A:809:ASP:OD1	1.72	0.90
1:A:377:ASN:ND2	1:A:379:ASP:H	1.69	0.88
1:A:533:MET:HE3	2:B:38:LEU:HD21	1.56	0.87
1:A:785:PRO:HD2	3:A:1189:HOH:O	1.75	0.86
1:A:614:MET:O	1:A:618:THR:HG22	1.77	0.85
1:A:206:LYS:HB2	3:A:1170:HOH:O	1.77	0.84
1:A:514:THR:CG2	1:A:557:ARG:HH12	1.91	0.83
1:A:707:ARG:HD3	1:A:757:TYR:CG	2.13	0.83
1:A:234:ARG:HD3	3:A:1171:HOH:O	1.78	0.83
1:A:369:PRO:HG2	3:A:980:HOH:O	1.79	0.82
1:A:323:VAL:N	1:A:324:PRO:HD2	1.94	0.82
1:A:777:LYS:CG	1:A:778:GLY:N	2.42	0.81
1:A:88:ARG:HH12	1:A:125:GLN:HG2	1.42	0.81
1:A:707:ARG:CD	1:A:757:TYR:CG	2.64	0.81
1:A:685:ILE:O	1:A:685:ILE:HD13	1.79	0.81
1:A:678:CYS:SG	1:A:720:ILE:HD13	2.20	0.81
1:A:115:GLY:HA3	3:A:1196:HOH:O	1.78	0.81
1:A:331:THR:CG2	3:A:1174:HOH:O	2.29	0.80
1:A:618:THR:HG23	1:A:619:ALA:N	1.97	0.80
1:A:35:THR:HG23	3:A:1187:HOH:O	1.80	0.80
1:A:707:ARG:HD2	1:A:757:TYR:CE1	2.16	0.80
1:A:857:LYS:CB	1:A:860:THR:OG1	2.30	0.80
1:A:478:ALA:CB	1:A:535:ILE:HD13	2.11	0.80
1:A:707:ARG:CD	1:A:757:TYR:CE1	2.66	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:ARG:O	1:A:19:GLU:HG2	1.81	0.79
1:A:702:ASN:HD22	1:A:703:GLU:CG	1.97	0.78
1:A:377:ASN:HD22	1:A:379:ASP:H	1.28	0.78
1:A:162:ASP:OD2	1:A:163:PRO:CD	2.31	0.78
1:A:594:LYS:HG3	1:A:594:LYS:O	1.84	0.78
1:A:744:GLN:O	1:A:746:GLN:HG3	1.84	0.78
1:A:35:THR:CG2	3:A:1187:HOH:O	2.30	0.78
1:A:835:LYS:HG3	3:A:1204:HOH:O	1.83	0.78
1:A:488:ALA:HB3	1:A:489:ASP:OD1	1.83	0.78
1:A:530:GLU:OE1	2:B:38:LEU:CD2	2.32	0.77
1:A:734:VAL:HG23	3:A:941:HOH:O	1.83	0.77
1:A:488:ALA:CB	1:A:489:ASP:HA	2.15	0.77
1:A:783:VAL:O	1:A:785:PRO:CD	2.33	0.77
1:A:599:ASP:O	1:A:603:ILE:HD13	1.85	0.76
1:A:530:GLU:OE1	2:B:38:LEU:HD22	1.85	0.76
1:A:860:THR:O	1:A:863:THR:CG2	2.32	0.76
1:A:112:CYS:O	1:A:116:ILE:HD13	1.86	0.76
1:A:377:ASN:HD22	1:A:378:PRO:N	1.84	0.76
1:A:593:ARG:HG3	1:A:593:ARG:NH1	1.94	0.75
1:A:174:LEU:O	1:A:178:ILE:HD13	1.85	0.75
1:A:619:ALA:CB	1:A:623:GLY:HA3	2.15	0.75
1:A:173:ILE:O	1:A:177:ILE:HD13	1.85	0.75
1:A:855:THR:CG2	1:A:856:ASN:N	2.30	0.75
1:A:441:GLU:HG3	3:A:962:HOH:O	1.87	0.74
1:A:778:GLY:CA	1:A:781:GLU:OE2	2.35	0.74
1:A:104:TYR:HB2	3:A:975:HOH:O	1.87	0.74
1:A:71:ASP:OD2	1:A:704:ASN:HB2	1.87	0.74
1:A:860:THR:C	1:A:863:THR:HG22	2.06	0.74
1:A:857:LYS:HA	1:A:860:THR:H	1.53	0.74
1:A:511:LEU:O	1:A:514:THR:CG2	2.36	0.74
1:A:487:VAL:HG23	1:A:488:ALA:O	1.87	0.74
2:B:37:SER:O	2:B:38:LEU:CD1	2.35	0.73
1:A:719:ASP:OD1	2:B:55:ARG:HD3	1.88	0.73
1:A:27:ARG:NH2	3:A:950:HOH:O	2.22	0.73
1:A:664:TYR:CZ	1:A:706:HIS:CE1	2.77	0.72
1:A:407:ILE:HD11	1:A:442:ALA:HA	1.71	0.72
1:A:543:CYS:C	1:A:545:PRO:HD2	2.10	0.72
1:A:444:ILE:O	1:A:444:ILE:HG22	1.88	0.72
1:A:593:ARG:CG	1:A:593:ARG:NH1	2.45	0.72
1:A:368:LEU:N	1:A:369:PRO:HD2	2.05	0.72
3:A:1207:HOH:O	2:B:31:TYR:CD1	2.42	0.71
1:A:342:TRP:CE2	2:B:26:PRO:HD2	2.24	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:ASP:HB2	1:A:704:ASN:HD22	1.54	0.71
1:A:130:ILE:N	1:A:131:PRO:HD2	2.06	0.71
1:A:342:TRP:CD1	2:B:26:PRO:HD3	2.25	0.71
1:A:544:TYR:N	1:A:545:PRO:CD	2.52	0.70
1:A:707:ARG:HD3	1:A:757:TYR:CE2	2.25	0.70
1:A:105:ARG:HB3	1:A:106:PRO:HD2	1.74	0.70
1:A:618:THR:HG23	1:A:619:ALA:H	1.57	0.70
1:A:800:PHE:O	1:A:804:ILE:HG12	1.92	0.70
1:A:328:GLN:O	1:A:331:THR:HB	1.92	0.70
1:A:486:ASP:CG	1:A:486:ASP:O	2.30	0.69
1:A:422:VAL:CG2	3:A:1180:HOH:O	2.40	0.69
1:A:514:THR:HG21	1:A:557:ARG:NH1	2.02	0.69
1:A:535:ILE:O	1:A:535:ILE:HD12	1.93	0.68
1:A:364:VAL:N	1:A:365:PRO:HD2	2.09	0.67
1:A:343:ASN:HD22	1:A:343:ASN:C	1.98	0.67
1:A:676:ASP:HA	1:A:679:ARG:NH1	2.10	0.67
1:A:428:ALA:O	1:A:432:VAL:HG23	1.95	0.67
1:A:702:ASN:ND2	1:A:703:GLU:CG	2.56	0.66
2:B:37:SER:O	2:B:38:LEU:HD12	1.96	0.66
1:A:702:ASN:CB	1:A:703:GLU:CG	2.33	0.66
1:A:68:LYS:HD2	1:A:68:LYS:N	2.00	0.66
1:A:693:MET:CE	1:A:720:ILE:HG21	2.26	0.66
1:A:121:ILE:N	1:A:122:PRO:HD2	2.11	0.66
1:A:1:MET:HG2	1:A:2:GLU:H	1.60	0.66
1:A:696:LEU:HD22	1:A:713:ILE:HD12	1.78	0.65
1:A:167:GLN:HG3	1:A:204:PHE:HB2	1.79	0.65
1:A:784:HIS:N	1:A:785:PRO:CD	2.52	0.65
1:A:204:PHE:CD2	3:A:1172:HOH:O	2.49	0.65
1:A:702:ASN:O	1:A:705:VAL:CG2	2.31	0.65
1:A:693:MET:HE1	1:A:720:ILE:HG21	1.79	0.64
1:A:67:SER:HB2	3:A:1161:HOH:O	1.97	0.64
2:B:41:SER:O	2:B:45:ARG:HG3	1.97	0.64
1:A:744:GLN:O	1:A:746:GLN:CG	2.46	0.64
1:A:811:THR:CG2	1:A:814:VAL:HG23	2.27	0.64
1:A:812:ASP:OD2	1:A:854:LYS:HB3	1.98	0.63
1:A:105:ARG:CB	1:A:106:PRO:CD	2.62	0.63
1:A:857:LYS:H	1:A:859:LYS:HD3	1.64	0.63
1:A:619:ALA:HA	1:A:621:SER:N	2.08	0.63
3:A:1073:HOH:O	2:B:26:PRO:HG2	1.98	0.62
1:A:618:THR:O	1:A:621:SER:HB2	2.00	0.62
1:A:501:SER:HB3	3:A:1121:HOH:O	2.00	0.62
1:A:664:TYR:CE1	1:A:706:HIS:ND1	2.68	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:PHE:HD2	3:A:1172:HOH:O	1.83	0.61
1:A:856:ASN:C	1:A:857:LYS:CG	2.62	0.61
1:A:856:ASN:O	1:A:857:LYS:CG	2.42	0.61
1:A:859:LYS:HG2	1:A:860:THR:N	2.15	0.61
3:A:1207:HOH:O	2:B:31:TYR:HD1	1.81	0.61
1:A:227:GLN:NE2	1:A:263:ILE:HD12	2.14	0.61
1:A:588:LEU:HA	1:A:591:VAL:HG22	1.82	0.61
1:A:850:GLY:O	1:A:859:LYS:HA	2.00	0.60
1:A:323:VAL:N	1:A:324:PRO:CD	2.64	0.60
1:A:608:MET:CE	1:A:635:LEU:HD23	2.30	0.60
1:A:594:LYS:O	1:A:594:LYS:CG	2.49	0.60
1:A:745:ALA:C	1:A:746:GLN:HG3	2.21	0.60
1:A:257:GLY:N	1:A:258:PRO:HD2	2.16	0.60
1:A:744:GLN:O	1:A:746:GLN:NE2	2.32	0.60
1:A:204:PHE:HA	3:A:1170:HOH:O	2.01	0.59
1:A:261:PHE:O	1:A:265:ILE:HD13	2.02	0.59
1:A:464:PRO:HB2	1:A:522:ASN:HD22	1.68	0.59
1:A:702:ASN:HB3	1:A:703:GLU:CB	2.28	0.59
1:A:71:ASP:HB2	1:A:704:ASN:ND2	2.16	0.59
1:A:343:ASN:ND2	1:A:346:LYS:H	2.00	0.59
1:A:178:ILE:HG21	1:A:217:PHE:CE2	2.37	0.59
1:A:18:LEU:HD23	1:A:18:LEU:C	2.23	0.59
1:A:533:MET:HG2	1:A:590:ASN:HD22	1.68	0.59
1:A:668:LEU:HD13	1:A:709:VAL:HG22	1.84	0.59
2:B:31:TYR:CE2	2:B:32:LYS:HD2	2.38	0.59
1:A:762:ARG:CZ	1:A:804:ILE:HD12	2.33	0.58
1:A:664:TYR:CE1	1:A:706:HIS:CE1	2.92	0.58
1:A:626:GLU:C	1:A:626:GLU:OE1	2.42	0.58
1:A:205:THR:HA	1:A:208:ASN:HD22	1.67	0.58
1:A:441:GLU:CG	3:A:962:HOH:O	2.48	0.58
1:A:618:THR:CG2	3:A:1168:HOH:O	2.50	0.58
1:A:815:VAL:HG13	1:A:846:LEU:HD11	1.84	0.58
1:A:665:GLN:OE1	1:A:665:GLN:HA	2.03	0.58
1:A:422:VAL:HG23	3:A:897:HOH:O	2.04	0.58
1:A:608:MET:HE1	1:A:635:LEU:HD23	1.85	0.58
1:A:860:THR:HA	1:A:863:THR:HG22	1.86	0.57
1:A:174:LEU:HD22	1:A:178:ILE:HD11	1.86	0.57
1:A:676:ASP:HA	1:A:679:ARG:HH12	1.69	0.57
1:A:618:THR:HG21	3:A:1168:HOH:O	2.03	0.57
1:A:377:ASN:C	1:A:377:ASN:HD22	2.07	0.57
1:A:664:TYR:O	1:A:668:LEU:HB2	2.05	0.57
1:A:571:THR:O	1:A:575:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:751:ASP:OD1	1:A:752:TYR:N	2.38	0.57
1:A:860:THR:CA	1:A:863:THR:HG22	2.34	0.57
1:A:397:PRO:CB	1:A:402:LEU:HD11	2.18	0.57
1:A:364:VAL:N	1:A:365:PRO:CD	2.67	0.56
1:A:618:THR:CG2	1:A:619:ALA:N	2.67	0.56
1:A:653:PHE:HA	1:A:656:ILE:HG22	1.86	0.56
1:A:18:LEU:HD23	1:A:18:LEU:O	2.05	0.56
2:B:48:LEU:CD2	3:B:66:HOH:O	2.53	0.56
1:A:840:ARG:HB2	1:A:843:ILE:HD12	1.88	0.56
1:A:783:VAL:HG22	1:A:784:HIS:H	1.71	0.56
1:A:544:TYR:OH	1:A:596:GLN:HG3	2.05	0.56
1:A:533:MET:CG	1:A:587:THR:HA	2.36	0.56
1:A:182:ARG:HB3	3:A:1117:HOH:O	2.04	0.55
1:A:863:THR:HG23	1:A:864:TRP:N	2.20	0.55
1:A:511:LEU:C	1:A:514:THR:HG22	2.25	0.55
1:A:305:ARG:HH11	1:A:305:ARG:CB	2.20	0.55
1:A:32:ASN:HD22	1:A:34:PRO:HD2	1.71	0.55
1:A:234:ARG:CD	3:A:1171:HOH:O	2.44	0.55
1:A:762:ARG:NH1	1:A:804:ILE:HD12	2.21	0.55
1:A:853:SER:HA	1:A:854:LYS:C	2.27	0.55
1:A:80:TRP:O	1:A:88:ARG:HD3	2.07	0.55
1:A:162:ASP:OD2	1:A:163:PRO:N	2.40	0.55
1:A:161:ILE:HG21	1:A:166:LEU:CD1	2.37	0.55
1:A:614:MET:O	1:A:618:THR:CG2	2.52	0.54
1:A:157:ILE:O	1:A:161:ILE:HG22	2.07	0.54
1:A:130:ILE:N	1:A:131:PRO:CD	2.70	0.54
1:A:818:ALA:O	1:A:822:ILE:HG12	2.06	0.54
1:A:615:PHE:HB3	1:A:653:PHE:CE1	2.42	0.54
1:A:88:ARG:HH12	1:A:125:GLN:CG	2.15	0.54
1:A:488:ALA:CB	1:A:489:ASP:OD1	2.56	0.54
1:A:105:ARG:CB	1:A:106:PRO:HD3	2.24	0.54
1:A:226:THR:O	1:A:234:ARG:HG2	2.07	0.54
1:A:560:GLN:O	1:A:564:MET:HG3	2.07	0.54
1:A:590:ASN:O	1:A:593:ARG:HB2	2.07	0.54
1:A:860:THR:HA	1:A:863:THR:CG2	2.38	0.54
1:A:161:ILE:HD13	1:A:166:LEU:HG	1.90	0.54
1:A:514:THR:OG1	1:A:529:TYR:CE2	2.60	0.53
1:A:257:GLY:N	1:A:258:PRO:CD	2.71	0.53
1:A:853:SER:HA	1:A:854:LYS:O	2.08	0.53
1:A:530:GLU:OE1	2:B:38:LEU:HD21	2.05	0.53
1:A:368:LEU:N	1:A:369:PRO:CD	2.72	0.53
1:A:65:LEU:HD13	1:A:116:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:497:TYR:CZ	1:A:499:LEU:HB2	2.44	0.53
1:A:795:GLU:HB3	3:A:907:HOH:O	2.09	0.53
1:A:335:GLU:HB2	3:A:985:HOH:O	2.08	0.53
1:A:422:VAL:HG23	3:A:1180:HOH:O	2.07	0.53
1:A:560:GLN:HG2	1:A:564:MET:CE	2.38	0.53
1:A:791:GLN:N	1:A:792:PRO:HD2	2.24	0.52
1:A:702:ASN:HB3	1:A:703:GLU:HG3	0.62	0.52
1:A:520:HIS:HB3	3:A:901:HOH:O	2.09	0.52
1:A:497:TYR:HD1	1:A:500:SER:HG	1.55	0.52
1:A:164:GLU:C	3:A:1175:HOH:O	2.48	0.52
1:A:807:ASP:O	1:A:810:HIS:CD2	2.62	0.52
1:A:762:ARG:HD3	1:A:804:ILE:HD12	1.90	0.52
1:A:707:ARG:HD3	1:A:757:TYR:CD1	2.34	0.52
1:A:758:LEU:O	1:A:762:ARG:HG3	2.10	0.52
1:A:383:ARG:O	1:A:387:VAL:HG23	2.10	0.52
1:A:811:THR:CG2	1:A:814:VAL:CG2	2.88	0.51
1:A:38:VAL:O	1:A:42:ARG:HG3	2.10	0.51
1:A:707:ARG:HD3	1:A:757:TYR:CZ	2.46	0.51
1:A:4:ILE:O	1:A:8:GLU:HG3	2.09	0.51
1:A:445:ASN:OD1	1:A:447:VAL:N	2.41	0.51
1:A:364:VAL:HB	1:A:365:PRO:HD3	1.92	0.51
1:A:1:MET:HG2	1:A:2:GLU:N	2.24	0.51
1:A:398:GLU:O	1:A:402:LEU:HD13	2.11	0.51
1:A:112:CYS:O	1:A:116:ILE:CD1	2.58	0.51
1:A:252:MET:HA	1:A:252:MET:CE	2.41	0.51
1:A:202:LEU:HD12	1:A:243:LYS:HD3	1.93	0.51
1:A:815:VAL:HG13	1:A:846:LEU:CD1	2.40	0.50
1:A:555:MET:CE	1:A:603:ILE:HG13	2.41	0.50
1:A:407:ILE:CD1	1:A:442:ALA:HA	2.40	0.50
1:A:570:SER:HB2	3:A:1111:HOH:O	2.11	0.50
1:A:84:ASP:OD2	1:A:86:ASN:HB2	2.11	0.50
1:A:618:THR:CG2	1:A:619:ALA:H	2.24	0.50
1:A:65:LEU:HD13	1:A:116:ILE:HD11	1.93	0.50
1:A:88:ARG:NH1	1:A:125:GLN:HG2	2.21	0.50
1:A:117:ALA:O	1:A:121:ILE:HG12	2.12	0.50
1:A:227:GLN:HE21	1:A:263:ILE:HD12	1.75	0.50
1:A:560:GLN:HG2	1:A:564:MET:HE2	1.94	0.50
1:A:619:ALA:CB	1:A:623:GLY:CA	2.88	0.49
2:B:37:SER:OG	2:B:38:LEU:CD1	2.60	0.49
1:A:567:HIS:CD2	3:A:957:HOH:O	2.65	0.49
1:A:615:PHE:HA	1:A:618:THR:HG22	1.94	0.49
1:A:806:GLY:HA2	1:A:842:MET:CE	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:833:VAL:O	1:A:837:VAL:HG23	2.12	0.49
1:A:402:LEU:N	1:A:402:LEU:HD12	2.27	0.49
1:A:422:VAL:HG21	3:A:1180:HOH:O	2.09	0.49
1:A:339:ASP:HA	3:A:1067:HOH:O	2.11	0.49
1:A:648:GLU:HB2	3:A:1136:HOH:O	2.11	0.49
1:A:367:VAL:HG12	1:A:371:ILE:CD1	2.42	0.49
1:A:71:ASP:CB	1:A:704:ASN:HD22	2.23	0.49
1:A:305:ARG:HH11	1:A:305:ARG:HB3	1.78	0.49
1:A:151:LEU:HD23	1:A:154:ILE:HD12	1.94	0.49
1:A:783:VAL:HG22	1:A:784:HIS:N	2.28	0.48
1:A:342:TRP:CG	2:B:26:PRO:CD	2.95	0.48
2:B:59:VAL:HG12	2:B:63:ARG:HE	1.78	0.48
1:A:211:LYS:HD2	1:A:214:GLU:OE1	2.13	0.48
1:A:782:ASN:ND2	1:A:782:ASN:N	2.61	0.48
2:B:38:LEU:HB3	2:B:43:ARG:HH21	1.78	0.48
1:A:489:ASP:O	1:A:490:ASP:OD1	2.31	0.48
1:A:343:ASN:HD21	1:A:345:CYS:HB3	1.79	0.48
1:A:1:MET:CG	1:A:2:GLU:H	2.23	0.48
1:A:831:LYS:CG	1:A:831:LYS:O	2.61	0.48
1:A:357:THR:HG22	1:A:395:GLU:HG2	1.95	0.48
1:A:827:THR:HG21	3:B:76:HOH:O	2.14	0.48
1:A:567:HIS:HD2	3:A:957:HOH:O	1.95	0.47
1:A:227:GLN:NE2	1:A:263:ILE:CD1	2.77	0.47
2:B:38:LEU:HB3	2:B:43:ARG:NH2	2.29	0.47
1:A:664:TYR:CZ	1:A:706:HIS:ND1	2.82	0.47
1:A:749:LYS:HG3	1:A:749:LYS:O	2.14	0.47
1:A:306:PRO:HA	3:A:1165:HOH:O	2.14	0.47
1:A:707:ARG:CD	1:A:757:TYR:CZ	2.97	0.47
1:A:305:ARG:NH1	1:A:305:ARG:HB3	2.30	0.47
1:A:659:LYS:HB2	1:A:659:LYS:HE3	1.73	0.47
1:A:863:THR:CG2	1:A:864:TRP:N	2.77	0.47
1:A:86:ASN:HB3	3:A:1150:HOH:O	2.15	0.47
1:A:337:ASP:HA	3:A:1208:HOH:O	2.16	0.46
2:B:32:LYS:O	2:B:33:SER:C	2.53	0.46
1:A:121:ILE:N	1:A:122:PRO:CD	2.78	0.46
1:A:403:LYS:N	1:A:404:PRO:HD2	2.30	0.46
1:A:338:ASP:C	1:A:340:ASP:H	2.18	0.46
1:A:651:LYS:HD3	1:A:691:GLU:OE2	2.14	0.46
1:A:702:ASN:CG	1:A:703:GLU:CG	2.82	0.46
1:A:626:GLU:HG2	1:A:666:VAL:HA	1.98	0.46
1:A:831:LYS:O	1:A:831:LYS:HG2	2.14	0.46
1:A:626:GLU:HG3	3:A:1006:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:ILE:O	1:A:161:ILE:CG2	2.63	0.46
1:A:840:ARG:HG2	1:A:840:ARG:HH11	1.81	0.46
1:A:628:ALA:O	1:A:631:ALA:HB3	2.15	0.46
1:A:615:PHE:HB3	1:A:653:PHE:CZ	2.51	0.46
1:A:367:VAL:HG12	1:A:371:ILE:HD11	1.98	0.46
1:A:568:ILE:HA	3:A:1166:HOH:O	2.15	0.45
1:A:696:LEU:HD22	1:A:713:ILE:CD1	2.45	0.45
1:A:665:GLN:NE2	2:B:44:ARG:NH1	2.63	0.45
1:A:73:LYS:HE3	3:A:954:HOH:O	2.16	0.45
1:A:660:ASN:O	1:A:667:CYS:HB2	2.17	0.45
1:A:393:ILE:O	1:A:393:ILE:HD12	2.16	0.45
2:B:37:SER:OG	2:B:38:LEU:HD11	2.16	0.45
1:A:178:ILE:HG21	1:A:217:PHE:CZ	2.51	0.45
1:A:130:ILE:HG22	1:A:131:PRO:N	2.31	0.45
1:A:549:LYS:O	1:A:553:VAL:HG23	2.17	0.45
1:A:343:ASN:ND2	1:A:343:ASN:C	2.69	0.45
1:A:857:LYS:HB3	1:A:860:THR:HG1	1.78	0.45
1:A:488:ALA:HB1	1:A:489:ASP:CA	2.26	0.45
1:A:181:MET:HE1	1:A:198:LEU:HD22	1.99	0.45
1:A:533:MET:HE3	2:B:38:LEU:CD2	2.38	0.45
1:A:762:ARG:CZ	1:A:804:ILE:CD1	2.95	0.45
1:A:811:THR:HG23	1:A:814:VAL:HG23	1.99	0.45
1:A:360:GLU:O	1:A:363:ILE:HG22	2.16	0.45
1:A:209:PHE:CZ	1:A:244:ILE:HD12	2.52	0.45
2:B:27:ARG:HB3	2:B:30:GLN:OE1	2.17	0.45
1:A:778:GLY:HA3	1:A:781:GLU:CD	2.34	0.44
1:A:532:LEU:O	1:A:535:ILE:HG22	2.16	0.44
1:A:840:ARG:HB2	1:A:843:ILE:CD1	2.46	0.44
1:A:425:ARG:NH2	1:A:463:GLU:OE1	2.50	0.44
1:A:591:VAL:HG23	1:A:592:LEU:N	2.33	0.44
1:A:693:MET:HG2	1:A:731:TYR:CD1	2.52	0.44
1:A:497:TYR:CD1	1:A:497:TYR:C	2.90	0.44
1:A:27:ARG:O	1:A:31:GLU:HG3	2.17	0.44
1:A:121:ILE:H	1:A:122:PRO:HD2	1.80	0.44
2:B:38:LEU:N	2:B:38:LEU:CD1	2.42	0.44
1:A:162:ASP:CG	1:A:163:PRO:HD2	2.36	0.44
1:A:158:CYS:SG	1:A:204:PHE:HZ	2.41	0.44
1:A:623:GLY:CA	3:A:1028:HOH:O	2.66	0.44
1:A:331:THR:HG23	3:A:1174:HOH:O	2.07	0.44
1:A:116:ILE:HD12	1:A:116:ILE:N	2.32	0.44
1:A:679:ARG:HH21	2:B:55:ARG:HG3	1.81	0.44
1:A:406:VAL:HG21	1:A:439:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:618:THR:O	1:A:621:SER:CB	2.63	0.43
1:A:615:PHE:HA	1:A:618:THR:CG2	2.48	0.43
1:A:139:ASN:HB3	1:A:142:SER:OG	2.18	0.43
1:A:36:PHE:CZ	1:A:40:LEU:HD11	2.54	0.43
1:A:495:ALA:HA	1:A:541:LYS:HG3	2.01	0.43
1:A:162:ASP:OD2	1:A:162:ASP:C	2.56	0.43
1:A:178:ILE:HG23	1:A:221:VAL:HG21	2.01	0.43
1:A:380:TRP:CZ2	1:A:381:ARG:NH1	2.87	0.43
1:A:430:TRP:CZ2	1:A:434:ARG:CD	3.01	0.43
1:A:533:MET:HG3	1:A:587:THR:HA	2.01	0.43
1:A:105:ARG:HA	1:A:105:ARG:HD2	1.71	0.43
1:A:515:ASP:OD2	1:A:557:ARG:NH2	2.51	0.43
1:A:33:LEU:HB3	1:A:34:PRO:HD3	2.00	0.43
1:A:157:ILE:HG22	1:A:166:LEU:HD11	2.00	0.43
1:A:782:ASN:HD22	1:A:782:ASN:N	2.16	0.43
1:A:752:TYR:O	1:A:755:VAL:HG12	2.18	0.43
1:A:588:LEU:HA	1:A:591:VAL:CG2	2.48	0.43
1:A:34:PRO:O	1:A:38:VAL:HG23	2.18	0.43
1:A:774:GLN:O	1:A:777:LYS:O	2.37	0.43
1:A:623:GLY:HA3	3:A:1028:HOH:O	2.18	0.43
1:A:121:ILE:HD11	1:A:129:LEU:HD23	2.01	0.43
1:A:797:ILE:O	1:A:801:ILE:HG12	2.18	0.43
1:A:287:CYS:O	1:A:291:MET:HG3	2.18	0.43
1:A:645:LYS:HG2	1:A:645:LYS:O	2.19	0.42
1:A:206:LYS:HE2	3:A:1170:HOH:O	2.19	0.42
1:A:343:ASN:HD21	1:A:346:LYS:H	1.66	0.42
2:B:52:LYS:HE2	3:B:71:HOH:O	2.18	0.42
1:A:250:GLN:HG3	3:A:1188:HOH:O	2.18	0.42
1:A:445:ASN:ND2	3:A:960:HOH:O	2.51	0.42
1:A:857:LYS:CA	1:A:860:THR:OG1	2.68	0.42
1:A:811:THR:HG23	1:A:814:VAL:H	1.83	0.42
1:A:73:LYS:O	1:A:77:GLN:HG3	2.20	0.42
1:A:711:PRO:HB3	1:A:761:LEU:HA	2.02	0.42
1:A:624:VAL:HG21	1:A:656:ILE:HG23	2.02	0.42
1:A:472:TRP:CD2	2:B:34:LYS:HG2	2.55	0.42
1:A:24:PHE:C	1:A:24:PHE:CD1	2.92	0.42
1:A:691:GLU:O	1:A:695:LEU:HG	2.19	0.42
1:A:630:MET:HG2	2:B:47:LEU:CD2	2.49	0.42
1:A:765:CYS:O	1:A:768:ALA:HB3	2.20	0.42
1:A:602:GLN:O	1:A:606:VAL:HG23	2.20	0.42
1:A:702:ASN:CG	1:A:703:GLU:HG2	2.39	0.41
1:A:402:LEU:N	1:A:402:LEU:CD1	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:LEU:HA	1:A:166:LEU:HD23	1.83	0.41
1:A:495:ALA:HA	1:A:541:LYS:CG	2.50	0.41
1:A:5:THR:O	1:A:9:LYS:HG2	2.19	0.41
1:A:812:ASP:OD2	1:A:854:LYS:CB	2.67	0.41
1:A:83:ILE:O	1:A:84:ASP:C	2.59	0.41
1:A:740:GLN:NE2	1:A:796:PHE:CZ	2.88	0.41
1:A:68:LYS:O	1:A:70:PRO:HD3	2.20	0.41
1:A:377:ASN:HD22	1:A:379:ASP:N	2.06	0.41
2:B:40:GLN:HG2	2:B:40:GLN:H	1.54	0.41
1:A:560:GLN:HG2	1:A:564:MET:HE1	2.03	0.41
1:A:161:ILE:HG21	1:A:166:LEU:HD12	2.02	0.41
1:A:68:LYS:CD	1:A:68:LYS:H	1.98	0.41
1:A:67:SER:CB	3:A:1161:HOH:O	2.63	0.41
1:A:806:GLY:HA2	1:A:842:MET:HE3	2.02	0.41
1:A:430:TRP:CZ2	1:A:434:ARG:HD3	2.56	0.41
1:A:702:ASN:HD22	1:A:703:GLU:HA	1.85	0.41
2:B:36:SER:C	2:B:38:LEU:N	2.74	0.41
1:A:800:PHE:CE1	1:A:804:ILE:HD11	2.55	0.41
1:A:853:SER:O	1:A:853:SER:OG	2.35	0.41
1:A:578:ASN:HA	1:A:578:ASN:HD22	1.68	0.41
1:A:253:GLU:OE1	1:A:312:LYS:HE3	2.20	0.41
1:A:853:SER:HB2	1:A:859:LYS:HB3	2.02	0.41
1:A:129:LEU:C	1:A:131:PRO:HD2	2.41	0.41
1:A:665:GLN:HE21	2:B:44:ARG:NH1	2.19	0.41
2:B:48:LEU:HD23	3:B:66:HOH:O	2.17	0.41
1:A:625:GLN:O	1:A:627:ASP:N	2.54	0.41
1:A:151:LEU:HA	1:A:154:ILE:HD12	2.03	0.40
1:A:466:VAL:O	1:A:470:VAL:HG23	2.21	0.40
1:A:759:ASN:HB3	1:A:811:THR:HG21	2.03	0.40
1:A:475:SER:O	1:A:479:GLU:HG3	2.21	0.40
1:A:809:ASP:OD1	1:A:809:ASP:N	2.50	0.40
1:A:444:ILE:O	1:A:444:ILE:CG2	2.60	0.40
2:B:50:LEU:HD11	2:B:54:LYS:NZ	2.36	0.40
1:A:737:ASN:O	1:A:740:GLN:HB3	2.22	0.40
1:A:253:GLU:HA	1:A:314:TYR:OH	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	871/876 (99%)	809 (93%)	58 (7%)	4 (0%)	38	45
2	B	37/40 (92%)	31 (84%)	6 (16%)	0	100	100
All	All	908/916 (99%)	840 (92%)	64 (7%)	4 (0%)	43	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	TYR
1	A	32	ASN
1	A	444	ILE
1	A	687	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	749/751 (100%)	691 (92%)	58 (8%)	18	20
2	B	38/39 (97%)	33 (87%)	5 (13%)	6	5
All	All	787/790 (100%)	724 (92%)	63 (8%)	17	19

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LEU
1	A	32	ASN
1	A	35	THR
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	67	SER
1	A	172	GLU
1	A	234	ARG
1	A	254	THR
1	A	305	ARG
1	A	331	THR
1	A	340	ASP
1	A	343	ASN
1	A	353	MET
1	A	377	ASN
1	A	413	LEU
1	A	417	MET
1	A	434	ARG
1	A	474	PHE
1	A	486	ASP
1	A	487	VAL
1	A	491	GLN
1	A	493	GLU
1	A	497	TYR
1	A	515	ASP
1	A	524	LEU
1	A	532	LEU
1	A	535	ILE
1	A	541	LYS
1	A	561	VAL
1	A	563	GLN
1	A	580	LEU
1	A	593	ARG
1	A	594	LYS
1	A	595	VAL
1	A	599	ASP
1	A	616	GLN
1	A	621	SER
1	A	625	GLN
1	A	626	GLU
1	A	637	GLU
1	A	654	LEU
1	A	673	LEU
1	A	685	ILE
1	A	690	ASP
1	A	707	ARG
1	A	746	GLN

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Mol	Chain	Res	Type
1	A	747	VAL
1	A	779	ASP
1	A	781	GLU
1	A	782	ASN
1	A	821	LEU
1	A	840	ARG
1	A	853	SER
1	A	855	THR
1	A	856	ASN
1	A	857	LYS
1	A	859	LYS
2	B	33	SER
2	B	38	LEU
2	B	40	GLN
2	B	54	LYS
2	B	61	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	32	ASN
1	A	49	ASN
1	A	141	ASN
1	A	145	HIS
1	A	179	GLN
1	A	208	ASN
1	A	227	GLN
1	A	240	ASN
1	A	278	GLN
1	A	320	GLN
1	A	343	ASN
1	A	377	ASN
1	A	401	GLN
1	A	408	GLN
1	A	522	ASN
1	A	578	ASN
1	A	581	GLN
1	A	590	ASN
1	A	702	ASN
1	A	704	ASN
1	A	712	GLN

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Mol	Chain	Res	Type
1	A	740	GLN
1	A	741	GLN
1	A	780	GLN
1	A	782	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	873/876 (99%)	0.38	59 (6%) 17 19	16, 42, 88, 160	0
2	B	39/40 (97%)	0.91	6 (15%) 3 3	34, 62, 104, 128	0
All	All	912/916 (99%)	0.41	65 (7%) 16 18	16, 42, 91, 160	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	780	GLN	20.8
1	A	783	VAL	10.1
1	A	487	VAL	9.9
1	A	488	ALA	9.7
1	A	490	ASP	9.1
1	A	489	ASP	9.0
1	A	778	GLY	8.0
1	A	779	ASP	8.0
1	A	782	ASN	8.0
2	B	38	LEU	7.3
1	A	491	GLN	6.6
1	A	748	ASP	6.6
1	A	704	ASN	6.5
1	A	750	SER	6.3
1	A	618	THR	5.6
1	A	749	LYS	5.6
1	A	486	ASP	5.6
1	A	854	LYS	4.8
2	B	40	GLN	4.6
1	A	746	GLN	4.4
1	A	104	TYR	4.2
1	A	492	GLU	4.1
1	A	752	TYR	4.0
1	A	784	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	856	ASN	3.6
1	A	702	ASN	3.6
2	B	35	TYR	3.5
1	A	855	THR	3.5
1	A	544	TYR	3.5
1	A	105	ARG	3.5
1	A	446	ASP	3.5
1	A	664	TYR	3.4
1	A	703	GLU	3.4
1	A	811	THR	3.4
2	B	37	SER	3.3
1	A	777	LYS	3.3
1	A	1	MET	3.1
1	A	103	THR	2.8
2	B	39	GLU	2.8
1	A	781	GLU	2.7
1	A	660	ASN	2.7
1	A	863	THR	2.7
1	A	621	SER	2.6
1	A	571	THR	2.6
1	A	753	ASP	2.5
1	A	661	TYR	2.5
1	A	844	HIS	2.5
1	A	454	GLN	2.5
1	A	163	PRO	2.4
1	A	619	ALA	2.4
1	A	803	HIS	2.3
1	A	593	ARG	2.3
1	A	853	SER	2.2
1	A	535	ILE	2.2
1	A	656	ILE	2.2
1	A	843	ILE	2.2
1	A	623	GLY	2.2
1	A	808	GLU	2.2
1	A	250	GLN	2.1
1	A	68	LYS	2.1
1	A	842	MET	2.1
1	A	755	VAL	2.1
1	A	754	MET	2.1
2	B	26	PRO	2.1
1	A	566	SER	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.