

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 4, 2024 – 07:22 AM EST

PDB ID	:	1NL3
Title	:	CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION
		ATPASE FROM MYCOBACTERIUM TUBERCULOSIS in APO FORM
Authors	:	Sharma, V.; Arockiasamy, A.; Ronning, D.R.; Savva, C.G.; Holzenburg, A.;
		Braunstein, M.; Jacobs Jr., W.R.; Sacchettini, J.C.; TB Structural Genomics
		Consortium (TBSGC)
Deposited on	:	2003-01-06
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
$\mathrm{EDS}$	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of	chain	
1	А	922	60%	25%	6% • 9%
1	В	922	56%	27%	7% • 9%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14209 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	А	839	Total 6639	C 4157	N 1169	0 1288	S 25	0	0	0
1	В	838	Total 6640	C 4157	N 1171	0 1287	S 25	0	0	0

• Molecule 1 is a protein called PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-29	MET	-	cloning artifact	UNP P0A5Y8
А	-28	LYS	-	cloning artifact	UNP P0A5Y8
А	-27	GLU	-	cloning artifact	UNP P0A5Y8
А	-26	THR	-	cloning artifact	UNP P0A5Y8
А	-25	ALA	-	cloning artifact	UNP P0A5Y8
А	-24	ALA	-	cloning artifact	UNP P0A5Y8
А	-23	ALA	-	cloning artifact	UNP P0A5Y8
А	-22	LYS	-	cloning artifact	UNP P0A5Y8
А	-21	PHE	-	cloning artifact	UNP P0A5Y8
А	-20	GLU	-	cloning artifact	UNP P0A5Y8
А	-19	ARG	-	cloning artifact	UNP P0A5Y8
А	-18	GLN	-	cloning artifact	UNP P0A5Y8
А	-17	HIS	-	cloning artifact	UNP P0A5Y8
А	-16	MET	-	cloning artifact	UNP P0A5Y8
А	-15	ASP	-	cloning artifact	UNP P0A5Y8
А	-14	SER	-	cloning artifact	UNP P0A5Y8
А	-13	PRO	-	cloning artifact	UNP P0A5Y8
А	-12	ASP	-	cloning artifact	UNP P0A5Y8
А	-11	LEU	-	cloning artifact	UNP P0A5Y8
А	-10	GLY	-	cloning artifact	UNP P0A5Y8
А	-9	THR	-	cloning artifact	UNP P0A5Y8
А	-8	LEU	-	cloning artifact	UNP P0A5Y8
А	-7	VAL	-	cloning artifact	UNP P0A5Y8
А	-6	PRO	-	cloning artifact	UNP P0A5Y8
А	A -5 ARG			cloning artifact	UNP P0A5Y8

There are 62 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	-4	GLY	-	cloning artifact	UNP P0A5Y8
А	-3	SER	-	cloning artifact	UNP P0A5Y8
А	-2	MET	-	cloning artifact	UNP P0A5Y8
А	-1	ALA	-	cloning artifact	UNP P0A5Y8
А	0	ASP	-	cloning artifact	UNP P0A5Y8
А	1	ILE	-	cloning artifact	UNP P0A5Y8
В	-29	MET	-	cloning artifact	UNP P0A5Y8
В	-28	LYS	-	cloning artifact	UNP P0A5Y8
В	-27	GLU	-	cloning artifact	UNP P0A5Y8
В	-26	THR	-	cloning artifact	UNP P0A5Y8
В	-25	ALA	-	cloning artifact	UNP P0A5Y8
В	-24	ALA	-	cloning artifact	UNP P0A5Y8
В	-23	ALA	-	cloning artifact	UNP P0A5Y8
В	-22	LYS	-	cloning artifact	UNP P0A5Y8
В	-21	PHE	-	cloning artifact	UNP P0A5Y8
В	-20	GLU	-	cloning artifact	UNP P0A5Y8
В	-19	ARG	-	cloning artifact	UNP P0A5Y8
В	-18	GLN	-	cloning artifact	UNP P0A5Y8
В	-17	HIS	-	cloning artifact	UNP P0A5Y8
В	-16	MET	-	cloning artifact	UNP P0A5Y8
В	-15	ASP	-	cloning artifact	UNP P0A5Y8
В	-14	SER	-	cloning artifact	UNP P0A5Y8
В	-13	PRO	-	cloning artifact	UNP P0A5Y8
В	-12	ASP	-	cloning artifact	UNP P0A5Y8
В	-11	LEU	-	cloning artifact	UNP P0A5Y8
В	-10	GLY	-	cloning artifact	UNP P0A5Y8
В	-9	THR	-	cloning artifact	UNP P0A5Y8
В	-8	LEU	-	cloning artifact	UNP P0A5Y8
В	-7	VAL	-	cloning artifact	UNP P0A5Y8
В	-6	PRO	-	cloning artifact	UNP P0A5Y8
В	-5	ARG	-	cloning artifact	UNP P0A5Y8
В	-4	GLY	-	cloning artifact	UNP P0A5Y8
В	-3	SER	-	cloning artifact	UNP P0A5Y8
В	-2	MET	-	cloning artifact	UNP P0A5Y8
В	-1	ALA	-	cloning artifact	UNP P0A5Y8
В	0	ASP	-	cloning artifact	UNP P0A5Y8
В	1	ILE	-	cloning artifact	UNP P0A5Y8

• Molecule 2 is water.

Mol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
2	А	475	Total 475	O 475	0	0
				$\alpha$	1	1

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	455	Total O 455 455	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT



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Chain B: 56% 27% 7% 9%



MET	LYS	THR	ALA	ALA ALA	LYS	GLU	ARG	SIH	MET	D-15 S-14	P-13	D-12	R-5	G-4		5	K4	Г2 - С	L6 R7	L8	010	7 TVI	K15	K18		A21	V24	-	D30 V31		T35 D36	-	L39 D40	A41	K42	T43 D44		R48 R49	L50	D52	053 K54
N55	DEA	FO J	L78	D79 080	R81	M88	TO THE	тоты	K107	T108	C111	V112	V116	L117	N118	T100	V130		Y 133	K1 <mark>36</mark>	R137	W141	M142	G143 R144	V145	H146 B147	L14/ F148		L151 0152		V155	D163	DIGE		N178	N179	D184	Y185 1.186		TAT	D1 <mark>95</mark> D196
-	R200	A205		V210 D211	<mark>\$212</mark>	D216	0104	AT 7A	L222	1223 1224	122 <del>1</del> S225	G226	P227 4728	D229		S232 ND33	W234	Y235	R240	L241	A242 D2/13	0441	E246	K247 D248	V249	H250 V261		D254	L255 B256	K257	R258 T259	V260	K O GE	0070	V270	1276	D277	N278	E281	N284	S289
Y290	L291	L295		E299	R303	V305	0061	R310	D311	<b>D</b> 318	E319	F320	1321 (1320	R323	V324	L325 T376	G327	R328	6754	<mark>ດ336</mark>	K3A1	E342		E345 T346	K347	A348 E240	E349 N350	Q351	T352 1.353	A354	T355 1356	T357	L358 D350	2 2 3	L364	Y365 D366	K367	M371	T372	A375	E381
-	E384	V391		M397	K410	E412	E413	D421	D422	V423	E425	R426	K429	G430		V433 1 A 3 A	1435	G436	143/ T438	S439	V440 E771	E111 R442	S443	E444	S447	R448	4443 F450		R453 R454	I455	P456 H457		L460	K463	Y464	E468		1472	R478	N486	G489
R490	2010	0	D501	D505	0506 0506	1 DOU	E510	TICN	D514	F617	T518	P519	E520 E521	Y522	E523	неот	S528	E529	L530 P531	1532	V533 KF34	E535	E536	A537 S538	K539	E540	E543		E546	Y551	V552	T555	E556 DE57	H558	E559	D564	N565	<b>q566</b>	R570	6572	R573
E579	TEOG	0001	R592	R593	L599 E600	<b>T601</b>	L602	1604	R605	T 608	P609	D610	F615	A616	K617	M618 V619	T620	R621	K624		0629 11630		E636	V637 B638	K639	MEAD	N649	<b>Q650</b>	0651 R652	K653	V654 I655		R659 D660	R661	I662	L663	K669	D670 0671	A672	D674	R677
D678	V693	V684	D685	G686 A687	T688	A693	E694	0690 N696	D697	L698 Deag	A700	L701	Wi7 02	L705		47.09	I713	T714	A/15 D716	S717	L718 T710	ARG	LYS	ASP HTS	GLU	PHE	ARG	ASP	ASP	THR	ARG E733	E734	L735	E737		L740 K741	D742	R750		L/ 34 E755	E756 I757
A758	G759 E760		M763	R764	E767	N769 N769	V770		V774	1775 D776	R777	K778	8780 8780		Y784	E785	Y788		E/91 G792	1793	G794 1 705	R796	A797	M798 4799	008b	R801 D802	P803		E806 Y807	0808	R809 E810		M814	D820	G821	M822 K823	E824	E825 S826	V827	F831	N832
V835	GLU AT A	VAL	PRO	ALA PRO	PRO	ALA	PRO	ALA ALA	GLU	PRO AT A	GLU	LEU	ALA	PHE	ALA	ALA AT A	ALA	ALA	ALA ALA	ALA	GLN GLN	ARG	SER	ALA VAL	ASP	GLY	ALA	ARG	GLU ARG	ALA	PR0 SER	ALA	LEU	ALA	LYS	GLY VAL	ALA	SER GLU	SER	ALA	



## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source		
Space group	P 62 2 2	Depositor		
Cell constants	206.20Å 206.20Å 295.41Å	Depositor		
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor		
Resolution (Å)	8.00 - 2.80	Depositor		
% Data completeness	99.4 (8.00-2.80)	Depositor		
(in resolution range)	33.4 (0.00 2.00)	Depositor		
$R_{merge}$	(Not available)	Depositor		
$R_{sym}$	0.10	Depositor		
Refinement program	REFMAC $5.1.25$	Depositor		
$R, R_{free}$	0.193 , $0.259$	Depositor		
Estimated twinning fraction	No twinning to report.	Xtriage		
Total number of atoms	14209	wwPDB-VP		
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP		



# 5 Model quality (i)

## 5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	B	ond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.59	0/6743	0.87	26/9116~(0.3%)
1	В	0.59	0/6744	0.88	25/9116~(0.3%)
All	All	0.59	0/13487	0.87	51/18232~(0.3%)

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	А	0	1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	В	820	ASP	CB-CG-OD2	7.49	125.04	118.30
1	В	79	ASP	CB-CG-OD2	7.42	124.98	118.30
1	А	248	ASP	CB-CG-OD2	7.18	124.76	118.30
1	А	820	ASP	CB-CG-OD2	6.83	124.45	118.30
1	А	318	ASP	CB-CG-OD2	6.68	124.31	118.30
1	В	716	ASP	CB-CG-OD2	6.66	124.29	118.30
1	А	645	ASP	CB-CG-OD2	6.65	124.29	118.30
1	В	685	ASP	CB-CG-OD2	6.58	124.22	118.30
1	А	678	ASP	CB-CG-OD2	6.38	124.04	118.30
1	А	306	ASP	CB-CG-OD2	6.26	123.94	118.30
1	А	674	ASP	CB-CG-OD2	6.23	123.91	118.30
1	А	216	ASP	CB-CG-OD2	6.22	123.90	118.30
1	А	172	ASP	CB-CG-OD2	6.20	123.88	118.30
1	В	184	ASP	CB-CG-OD2	6.12	123.80	118.30
1	А	79	ASP	CB-CG-OD2	6.09	123.78	118.30
1	А	84	ASP	CB-CG-OD2	6.02	123.72	118.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	674	ASP	CB-CG-OD2	6.01	123.71	118.30
1	А	813	ASP	CB-CG-OD2	5.73	123.46	118.30
1	В	364	LEU	CA-CB-CG	5.73	128.48	115.30
1	В	44	ASP	CB-CG-OD2	5.64	123.38	118.30
1	А	272	ASP	CB-CG-OD2	5.59	123.33	118.30
1	А	44	ASP	CB-CG-OD2	5.57	123.32	118.30
1	В	216	ASP	CB-CG-OD2	5.54	123.29	118.30
1	В	391	VAL	CB-CA-C	-5.51	100.93	111.40
1	В	-15	ASP	CB-CG-OD2	5.48	123.24	118.30
1	А	311	ASP	CB-CG-OD2	5.46	123.21	118.30
1	А	493	ASP	CB-CG-OD2	5.46	123.21	118.30
1	В	196	ASP	CB-CG-OD2	5.40	123.16	118.30
1	В	366	ASP	CB-CG-OD2	5.39	123.15	118.30
1	В	318	ASP	CB-CG-OD2	5.36	123.12	118.30
1	А	132	ASP	CB-CG-OD2	5.35	123.11	118.30
1	В	36	ASP	CB-CG-OD2	5.35	123.11	118.30
1	В	155	VAL	CB-CA-C	-5.35	101.24	111.40
1	В	30	ASP	CB-CG-OD2	5.32	123.09	118.30
1	В	610	ASP	CB-CG-OD2	5.29	123.06	118.30
1	А	-15	ASP	CB-CG-OD2	5.27	123.04	118.30
1	В	195	ASP	CB-CG-OD2	5.26	123.03	118.30
1	А	588	ASP	CB-CG-OD2	5.24	123.02	118.30
1	А	304	ASP	CB-CG-OD2	5.21	122.99	118.30
1	В	-12	ASP	CB-CG-OD2	5.17	122.96	118.30
1	А	210	VAL	CB-CA-C	-5.15	101.62	111.40
1	А	699	ASP	CB-CG-OD2	5.10	122.89	118.30
1	А	403	ASP	CB-CG-OD2	5.08	122.87	118.30
1	В	486	ASN	C-N-CA	-5.08	109.01	121.70
1	А	155	VAL	CB-CA-C	-5.06	101.79	111.40
1	В	699	ASP	CB-CG-OD2	5.05	122.84	118.30
1	В	505	ASP	CB-CG-OD2	5.04	122.83	118.30
1	В	564	ASP	CB-CG-OD2	5.03	122.82	118.30
1	В	742	ASP	CB-CG-OD2	5.02	122.82	118.30
1	А	695	ASP	CB-CG-OD2	5.02	122.81	118.30
1	А	30	ASP	CB-CG-OD2	5.01	122.81	118.30

Continued from previous page...

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	320	PHE	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	А	6639	0	6576	197	0
1	В	6640	0	6585	220	0
2	А	475	0	0	57	0
2	В	455	0	0	67	0
All	All	14209	0	13161	409	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (409) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:615:GLU:HG3	1:B:323:ARG:HG3	1.37	1.06
1:A:702:TRP:NE1	1:A:714:THR:HA	1.73	1.03
1:A:660:ARG:HG2	2:A:1748:HOH:O	1.60	1.01
1:B:359:GLN:H	1:B:359:GLN:HE21	1.08	1.00
1:A:734:GLU:O	1:A:735:LEU:HB3	1.64	0.94
1:B:141:TRP:HZ2	1:B:501:ASP:HB3	1.29	0.94
1:A:436:GLY:O	1:A:555:THR:HB	1.69	0.93
1:B:780:ARG:HD2	2:B:1298:HOH:O	1.70	0.92
1:A:702:TRP:HE1	1:A:714:THR:HA	1.34	0.91
1:A:359:GLN:H	1:A:359:GLN:HE21	1.04	0.91
1:A:777:ARG:NH2	1:A:825:GLU:OE1	2.03	0.90
1:B:755:GLU:HA	1:B:759:GLY:HA3	1.53	0.89
1:B:53:GLN:H	1:B:53:GLN:HE21	1.22	0.87
1:B:777:ARG:NH2	1:B:825:GLU:OE1	2.07	0.87
1:A:328:ARG:HG3	1:A:328:ARG:HH11	1.40	0.86
1:B:141:TRP:CZ2	1:B:501:ASP:HB3	2.11	0.86
1:A:421:ASP:OD1	1:A:453:ARG:NH2	2.09	0.85
1:A:806:GLU:HG3	2:A:1885:HOH:O	1.77	0.85
1:A:328:ARG:HH11	1:A:328:ARG:CG	1.92	0.82
1:B:447:SER:HB2	1:B:457:HIS:NE2	1.95	0.82
1:B:453:ARG:HG3	2:B:1847:HOH:O	1.81	0.81
1:A:384:GLU:HG3	2:A:1788:HOH:O	1.81	0.81
1:A:780:ARG:HD3	2:A:1593:HOH:O	1.79	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:246:GLU:H	1:A:250:HIS:HD2	1.29	0.80
1:B:3:SER:HB3	2:B:1795:HOH:O	1.82	0.80
1:B:558:HIS:HD2	1:B:564:ASP:OD2	1.65	0.79
2:A:1362:HOH:O	1:B:615:GLU:HG3	1.80	0.79
1:B:227:PRO:HD2	2:B:1863:HOH:O	1.83	0.79
1:B:683:TYR:HE2	2:B:1094:HOH:O	1.64	0.79
1:A:733:GLU:HA	2:A:1533:HOH:O	1.83	0.79
1:B:650:GLN:HG3	2:B:1306:HOH:O	1.81	0.79
1:A:734:GLU:HA	2:A:1698:HOH:O	1.84	0.77
1:A:246:GLU:H	1:A:250:HIS:CD2	2.03	0.76
1:B:191:ALA:O	1:B:659:ARG:NH2	2.18	0.76
1:B:558:HIS:CD2	1:B:564:ASP:OD2	2.39	0.76
1:A:558:HIS:HD2	1:A:564:ASP:OD2	1.70	0.75
1:B:759:GLY:O	1:B:760:GLU:HB2	1.85	0.75
1:A:86:GLN:HG2	1:A:110:THR:OG1	1.87	0.74
1:B:141:TRP:HE3	2:B:1713:HOH:O	1.71	0.73
1:B:705:LEU:HD23	1:B:709:TYR:CE1	2.24	0.73
1:B:705:LEU:HD23	1:B:709:TYR:HE1	1.52	0.73
1:B:636:GLU:HG3	2:B:1560:HOH:O	1.89	0.72
1:B:801:ARG:HD2	1:B:802:ASP:H	1.54	0.72
1:A:780:ARG:CD	2:A:1593:HOH:O	2.35	0.72
1:B:507:ARG:CG	1:B:507:ARG:HH11	2.03	0.71
1:B:592:ARG:HD2	2:B:1682:HOH:O	1.90	0.71
1:A:40:ARG:HG2	2:A:1665:HOH:O	1.90	0.71
1:A:144:ARG:HD2	1:A:523:GLU:OE2	1.91	0.70
1:A:780:ARG:HD2	2:A:1503:HOH:O	1.90	0.70
1:A:461:ASN:OD1	1:A:485:THR:HG21	1.92	0.69
1:A:611:ASP:HB3	2:A:1380:HOH:O	1.92	0.69
1:A:801:ARG:H	1:A:801:ARG:HE	1.38	0.69
1:A:461:ASN:HA	1:A:485:THR:HG23	1.73	0.69
1:A:381:GLU:OE1	1:A:638:ARG:NH1	2.25	0.69
1:A:75:TRP:HB2	1:A:81:ARG:HB2	1.75	0.69
1:A:669:LYS:HD3	1:A:764:ARG:NH2	2.08	0.68
1:B:246:GLU:HB3	1:B:249:VAL:HB	1.75	0.68
1:B:507:ARG:HD3	2:B:1832:HOH:O	1.91	0.68
1:A:764:ARG:HA	1:A:767:GLU:OE1	1.94	0.67
1:B:507:ARG:HH11	1:B:507:ARG:CB	2.07	0.67
1:B:775:ILE:HG12	1:B:822:MET:CE	2.24	0.67
1:B:714:THR:O	1:B:717:SER:HB2	1.93	0.67
1:A:615:GLU:CG	1:B:323:ARG:HG3	2.21	0.67
1:B:660:ARG:HG3	2:B:1740:HOH:O	1.94	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:570:ARG:HD2	2:B:1063:HOH:O	1.95	0.67
1:A:318:ASP:OD1	1:A:319:GLU:N	2.28	0.66
1:B:178:ASN:ND2	2:B:1702:HOH:O	2.23	0.66
1:A:741:LYS:HE3	2:A:1715:HOH:O	1.95	0.66
1:B:229:ASP:HB2	2:B:1746:HOH:O	1.96	0.66
1:B:179:ASN:HB2	2:B:1749:HOH:O	1.94	0.66
1:A:801:ARG:HE	1:A:801:ARG:N	1.92	0.66
1:A:15:LYS:HD3	2:A:1869:HOH:O	1.95	0.65
1:A:248:ASP:HA	2:A:1609:HOH:O	1.96	0.65
1:A:708:LEU:HD13	1:A:827:VAL:CG2	2.26	0.65
1:B:257:LYS:HG3	2:B:1639:HOH:O	1.97	0.65
1:A:326:ILE:HD13	1:B:608:LEU:HD12	1.79	0.65
1:A:546:GLU:HG3	2:A:1763:HOH:O	1.95	0.65
1:B:559:GLU:HG2	1:B:630:VAL:CG1	2.27	0.65
1:B:359:GLN:H	1:B:359:GLN:NE2	1.90	0.64
1:A:688:THR:O	1:A:688:THR:HG22	1.98	0.64
1:A:801:ARG:HD2	1:A:802:ASP:N	2.12	0.64
1:A:798:MET:HA	1:B:621:ARG:HH12	1.63	0.63
1:B:309:VAL:O	1:B:310:ARG:HD3	1.98	0.63
1:A:322:GLY:HA3	2:A:1642:HOH:O	1.98	0.63
1:B:490:ARG:HA	2:B:1818:HOH:O	1.99	0.63
1:B:801:ARG:HD2	1:B:802:ASP:N	2.14	0.63
1:B:511:ARG:NH2	1:B:529:GLU:OE2	2.32	0.62
1:B:4:LYS:C	1:B:6:LEU:H	2.01	0.62
1:A:668:LEU:HD13	1:A:771:LEU:HD12	1.80	0.62
1:B:80:GLN:HG2	2:B:1209:HOH:O	1.98	0.62
1:B:53:GLN:HE21	1:B:53:GLN:N	1.93	0.61
1:A:228:ALA:HB3	2:A:1405:HOH:O	2.00	0.61
1:A:326:ILE:HG13	1:A:327:GLY:N	2.15	0.61
1:A:632:GLN:HA	1:A:632:GLN:NE2	2.16	0.61
1:B:775:ILE:HG12	1:B:822:MET:HE2	1.81	0.61
1:B:806:GLU:HG2	2:B:1188:HOH:O	2.00	0.61
1:A:618:MET:HG3	2:B:1389:HOH:O	1.99	0.61
1:A:508:LEU:O	1:A:513:LEU:HB2	2.01	0.60
1:B:639:LYS:HD3	2:B:1438:HOH:O	1.99	0.60
1:B:683:TYR:CE2	2:B:1094:HOH:O	2.47	0.60
1:B:530:LEU:HB3	1:B:531:PRO:HD3	1.83	0.60
1:B:520:GLU:HG2	2:B:1911:HOH:O	2.02	0.60
1:B:429:LYS:HG2	2:B:1606:HOH:O	2.01	0.59
1:B:436:GLY:O	1:B:555:THR:HB	2.02	0.59
1:A:521:GLU:OE1	2:A:1766:HOH:O	2.16	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:440:VAL:O	1:B:444:GLU:HG2	2.03	0.59
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.14	0.59
1:A:246:GLU:HG3	2:A:1358:HOH:O	2.03	0.59
1:A:259:THR:HG23	2:A:1346:HOH:O	2.01	0.59
1:A:514:ASP:HB3	1:A:517:GLU:HB2	1.84	0.59
1:B:112:VAL:HG13	1:B:146:HIS:CE1	2.38	0.59
1:B:248:ASP:HA	2:B:1725:HOH:O	2.02	0.59
1:A:112:VAL:HG13	1:A:146:HIS:CE1	2.38	0.58
1:B:116:TYR:HD1	1:B:151:LEU:HD11	1.68	0.58
1:A:219:ARG:HB3	2:A:1874:HOH:O	2.02	0.58
1:A:461:ASN:HA	1:A:485:THR:CG2	2.34	0.58
1:B:797:ALA:HB1	1:B:801:ARG:HD3	1.86	0.58
1:B:116:TYR:CD1	1:B:151:LEU:HD11	2.39	0.58
1:B:357:THR:HB	1:B:359:GLN:NE2	2.18	0.58
1:B:426:ARG:HA	2:B:1813:HOH:O	2.03	0.58
1:A:539:LYS:HE2	2:A:1814:HOH:O	2.05	0.57
1:A:680:ILE:O	1:A:684:VAL:HG23	2.04	0.57
1:A:650:GLN:HG3	2:A:1371:HOH:O	2.05	0.57
1:B:254:ASP:CG	1:B:257:LYS:HB2	2.25	0.57
1:B:144:ARG:HD2	1:B:523:GLU:OE2	2.05	0.57
1:B:235:TYR:CE2	1:B:336:GLN:HG2	2.39	0.57
1:A:141:TRP:HZ2	2:A:1786:HOH:O	1.88	0.56
1:A:742:ASP:OD1	1:A:745:ARG:NH1	2.37	0.56
1:B:256:ARG:CB	1:B:256:ARG:HH11	2.18	0.56
1:B:39:LEU:HD23	1:B:148:PHE:HE1	1.70	0.56
1:A:410:LYS:HD2	1:A:603:LEU:HB3	1.86	0.56
1:B:108:THR:HG23	2:B:1651:HOH:O	2.04	0.56
1:B:256:ARG:HH11	1:B:256:ARG:HB2	1.71	0.56
1:A:245:MET:CE	1:A:270:VAL:HG22	2.37	0.55
1:B:649:ASN:HD22	1:B:652:ARG:HE	1.52	0.55
1:B:799:ALA:O	1:B:800:GLN:HB2	2.05	0.55
1:B:318:ASP:HB3	1:B:321:THR:HB	1.88	0.55
1:A:140:GLU:HA	1:A:147:ARG:HH22	1.71	0.55
1:B:359:GLN:HE21	1:B:359:GLN:N	1.92	0.55
1:B:137:ARG:HD2	2:B:1836:HOH:O	2.05	0.55
1:A:192:HIS:HD2	2:A:1694:HOH:O	1.89	0.55
1:A:233:ASN:HB3	2:A:1057:HOH:O	2.06	0.55
1:A:472:ILE:HG21	1:A:492:THR:HB	1.87	0.55
1:A:764:ARG:HD3	1:A:767:GLU:OE1	2.06	0.54
1:B:460:LEU:HB3	1:B:468:GLU:HG2	1.89	0.54
1:B:422:ASP:O	1:B:426:ARG:HG2	2.06	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:101:MET:HE3	1:A:371:MET:HE2	1.88	0.54
1:A:233:ASN:N	1:A:233:ASN:HD22	2.04	0.54
1:A:612:VAL:HG13	1:B:323:ABG:HH22	1.71	0.54
1.B.775.ILE.HG12	1.B.822.MET.HE3	1.90	0.54
1:A:245:MET:HE1	1:A:270:VAL:CG2	2.38	0.54
1:B:507:ARG:HH11	1:B:507:ARG:HG3	1.71	0.54
1:A:501:ASP:HB3	2:A:1786:HOH:O	2.07	0.54
1:A:243:PRO:HG2	2:A:1382:HOH:O	2.07	0.54
1:B:425:GLU:HG2	2:B:1707:HOH:O	2.07	0.54
1:A:328:ARG:HG3	1:A:328:ARG:NH1	2.17	0.54
1:A:793:ILE:HG22	2:A:1117:HOH:O	2.08	0.54
1:A:437:THR:HG22	1:A:555:THR:HG21	1.89	0.54
1:A:755:GLU:HB3	2:A:1925:HOH:O	2.08	0.54
1:B:4:LYS:C	1:B:6:LEU:N	2.62	0.54
1:B:429:LYS:HG3	2:B:1893:HOH:O	2.08	0.54
1:B:251:TYR:OH	1:B:299:GLU:OE2	2.18	0.53
1:A:662:ILE:HG21	1:A:772:LEU:HB2	1.90	0.53
1:B:303:ARG:O	1:B:304:ASP:HB2	2.08	0.53
1:B:53:GLN:H	1:B:53:GLN:NE2	2.00	0.53
1:B:694:GLU:O	1:B:696:TRP:N	2.41	0.53
1:B:801:ARG:HB3	2:B:1437:HOH:O	2.09	0.53
1:A:558:HIS:CD2	1:A:564:ASP:OD2	2.56	0.53
1:A:669:LYS:HD3	1:A:764:ARG:HH21	1.74	0.53
1:A:81:ARG:HD3	2:A:1319:HOH:O	2.08	0.53
1:B:801:ARG:NH2	2:B:1899:HOH:O	2.41	0.52
1:A:-14:SER:H	1:A:-3:SER:HB2	1.72	0.52
1:B:246:GLU:OE2	1:B:249:VAL:HG21	2.08	0.52
1:B:527:HIS:HB2	2:B:1513:HOH:O	2.08	0.52
1:B:447:SER:HA	1:B:450:PHE:HB2	1.91	0.52
1:B:684:VAL:O	1:B:688:THR:HB	2.10	0.52
1:B:372:THR:HG21	1:B:375:ALA:HB2	1.91	0.52
1:A:733:GLU:CB	2:A:1739:HOH:O	2.58	0.52
1:B:559:GLU:HG2	1:B:630:VAL:HG11	1.92	0.52
1:A:463:LYS:HB2	2:A:1859:HOH:O	2.09	0.52
1:B:246:GLU:H	1:B:250:HIS:HD2	1.57	0.51
1:A:329:ARG:HB3	1:A:335:HIS:CE1	2.45	0.51
1:A:490:ARG:NH1	2:A:1802:HOH:O	2.44	0.51
1:A:667:ASN:ND2	1:A:764:ARG:HD2	2.26	0.51
1:B:227:PRO:HA	1:B:349:GLU:O	2.10	0.51
1:B:243:PRO:HG2	2:B:1347:HOH:O	2.10	0.51
1:A:359:GLN:H	1:A:359:GLN:NE2	1.89	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:602:LEU:HD11	1:B:791:GLU:O	2.11	0.51
1:A:669:LYS:HE2	2:A:1860:HOH:O	2.10	0.51
1:A:708:LEU:HD13	1:A:827:VAL:HG22	1.92	0.51
1:A:289:SER:HB3	2:A:1842:HOH:O	2.09	0.51
1:A:240:ARG:O	1:A:243:PRO:HD2	2.11	0.51
1:A:675:MET:O	1:A:679:VAL:HG23	2.11	0.51
1:A:819:LEU:HD23	1:A:822:MET:CE	2.41	0.51
1:A:53:GLN:H	1:A:53:GLN:CD	2.14	0.51
1:A:693:ALA:C	1:A:695:ASP:H	2.15	0.51
1:B:228:ALA:HB3	2:B:1706:HOH:O	2.11	0.50
1:A:372:THR:CG2	1:A:375:ALA:HB2	2.40	0.50
1:B:278:ASN:HD21	1:B:832:ASN:ND2	2.09	0.50
1:B:118:ASN:HD21	1:B:367:LYS:NZ	2.10	0.50
1:B:129:THR:HB	2:B:1366:HOH:O	2.11	0.50
1:A:702:TRP:HE1	1:A:714:THR:CA	2.17	0.50
1:B:341:LYS:HE2	1:B:342:GLU:OE2	2.11	0.50
1:A:140:GLU:HA	1:A:147:ARG:NH2	2.26	0.50
1:A:328:ARG:CG	1:A:328:ARG:NH1	2.61	0.50
1:A:15:LYS:CD	2:A:1869:HOH:O	2.57	0.50
1:A:793:ILE:CG2	2:A:1117:HOH:O	2.60	0.50
1:B:810:GLU:O	1:B:814:MET:HG2	2.12	0.50
1:B:593:ARG:HD2	2:B:1701:HOH:O	2.10	0.50
1:B:660:ARG:CG	2:B:1740:HOH:O	2.57	0.50
1:B:136:LYS:HA	1:B:155:VAL:HG11	1.93	0.50
1:B:677:ARG:HD3	2:B:1289:HOH:O	2.11	0.50
1:A:254:ASP:HB3	1:A:259:THR:HG22	1.94	0.50
1:B:78:LEU:O	1:B:79:ASP:HB2	2.12	0.50
1:A:558:HIS:HE1	2:A:1297:HOH:O	1.93	0.49
1:A:258:ARG:HA	1:A:300:LEU:HD11	1.93	0.49
1:B:784:TYR:CE2	1:B:788:TYR:HE2	2.30	0.49
1:B:5:LEU:N	2:B:1569:HOH:O	2.45	0.49
1:B:42:LYS:NZ	2:B:1195:HOH:O	2.44	0.49
1:B:223:ILE:HG12	1:B:355:THR:HG22	1.95	0.49
1:A:101:MET:HE1	1:A:371:MET:HE3	1.94	0.49
1:B:733:GLU:O	1:B:735:LEU:N	2.46	0.49
1:A:715:ALA:O	1:A:717:SER:N	2.46	0.48
1:A:128:VAL:HA	1:A:176:GLY:O	2.13	0.48
1:B:254:ASP:HB3	1:B:259:THR:HG22	1.95	0.48
1:A:42:LYS:NZ	2:A:1285:HOH:O	2.46	0.48
1:A:490:ARG:HG2	2:A:1751:HOH:O	2.11	0.48
1:A:674:ASP:OD1	1:A:677:ARG:NH1	2.46	0.48



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:276:ILE:HG13	1:A:281:GLU:OE2	2.12	0.48
1:A:688:THR:HG23	1:A:696:TRP:CZ2	2.48	0.48
1:B:421:ASP:OD1	1:B:453:ARG:NH2	2.46	0.48
1:A:11:GLY:HA2	2:A:1133:HOH:O	2.13	0.48
1:A:357:THR:HB	1:A:359:GLN:NE2	2.29	0.48
1:B:453:ARG:CG	1:B:453:ARG:NH1	2.77	0.48
1:A:169:TYR:CZ	1:A:199:GLN:HG2	2.49	0.48
1:A:778:LYS:HE2	2:A:1431:HOH:O	2.14	0.48
1:B:328:ARG:HH11	1:B:796:ARG:HD2	1.79	0.47
1:B:372:THR:CG2	1:B:375:ALA:HB2	2.43	0.47
1:A:116:TYR:CZ	1:A:149:LEU:HD13	2.50	0.47
1:B:714:THR:O	1:B:717:SER:CB	2.61	0.47
1:B:2:LEU:C	1:B:4:LYS:H	2.18	0.47
1:B:472:ILE:HG13	1:B:489:GLY:HA3	1.97	0.47
1:B:764:ARG:HD3	1:B:764:ARG:HA	1.45	0.47
1:B:328:ARG:HG2	2:B:1598:HOH:O	2.14	0.47
1:B:648:MET:HG3	2:B:1537:HOH:O	2.14	0.47
1:B:345:GLU:HG3	2:B:1412:HOH:O	2.13	0.47
1:A:246:GLU:OE1	1:A:249:VAL:HG21	2.14	0.47
1:A:672:ALA:O	1:A:676:VAL:HG23	2.14	0.47
1:A:677:ARG:HD3	2:A:1341:HOH:O	2.14	0.47
1:B:24:VAL:HG22	1:B:64:PRO:HA	1.96	0.47
1:A:326:ILE:HG21	2:B:1884:HOH:O	2.14	0.47
1:B:15:LYS:HD3	2:B:1434:HOH:O	2.14	0.47
1:A:713:ILE:O	1:A:714:THR:O	2.32	0.47
1:B:321:THR:HG22	1:B:323:ARG:HB2	1.96	0.47
1:B:546:GLU:OE2	1:B:546:GLU:HA	2.15	0.47
1:A:509:ARG:HD2	2:A:1828:HOH:O	2.14	0.47
1:A:310:ARG:HA	1:A:310:ARG:HE	1.79	0.47
1:A:819:LEU:HD23	1:A:822:MET:HE2	1.97	0.47
1:B:543:GLU:HB3	2:B:1692:HOH:O	2.14	0.47
1:A:426:ARG:HD3	1:A:551:TYR:CD2	2.50	0.46
1:A:463:LYS:HE2	2:A:1768:HOH:O	2.14	0.46
1:A:75:TRP:CE2	2:A:1783:HOH:O	2.56	0.46
1:A:123:ASN:HB3	1:A:203:HIS:CD2	2.51	0.46
1:B:793:ILE:HG12	1:B:807:TYR:HB2	1.97	0.46
1:A:-5:ARG:HD3	1:A:-5:ARG:HA	1.65	0.46
1:A:233:ASN:H	1:A:233:ASN:ND2	2.14	0.46
1:A:647:VAL:HG22	1:A:808:GLN:HG3	1.97	0.46
1:A:191:ALA:O	1:A:659:ARG:NH2	2.38	0.46
1:B:716:ASP:O	1:B:717:SER:C	2.54	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:245:MET:HE1	1:A:270:VAL:HG22	1.96	0.46
1:B:12:ARG:NH1	2:B:1295:HOH:O	2.48	0.45
1:B:258:ARG:HG2	2:B:1493:HOH:O	2.15	0.45
1:B:662:ILE:HG23	1:B:768:ARG:HG2	1.97	0.45
1:A:226:GLY:O	1:A:350:ASN:HA	2.17	0.45
1:A:587:GLY:O	1:A:592:ARG:NH1	2.48	0.45
1:B:163:ASP:OD1	1:B:166:ARG:NH1	2.50	0.45
1:B:323:ARG:HD2	1:B:323:ARG:HA	1.73	0.45
1:B:39:LEU:O	1:B:40:ARG:CB	2.64	0.45
1:B:276:ILE:HG13	1:B:281:GLU:OE2	2.16	0.45
1:A:211:ASP:OD2	1:A:562:ARG:NH1	2.46	0.45
1:A:427:TYR:CZ	1:A:456:PRO:HD2	2.51	0.45
1:B:129:THR:CB	2:B:1366:HOH:O	2.64	0.45
1:B:444:GLU:HG2	1:B:444:GLU:H	1.64	0.45
1:A:372:THR:HG21	1:A:375:ALA:HB2	1.99	0.45
1:A:552:VAL:HG23	1:A:571:SER:HB2	1.97	0.45
1:B:4:LYS:HG3	2:B:1069:HOH:O	2.16	0.45
1:A:46:PHE:HB3	1:A:120:LEU:HD13	1.99	0.45
1:A:270:VAL:HG21	1:A:291:LEU:HD22	1.99	0.45
1:B:510:GLU:HG2	2:B:1916:HOH:O	2.17	0.45
1:A:359:GLN:HE21	1:A:359:GLN:N	1.89	0.45
1:A:546:GLU:HB3	2:A:1726:HOH:O	2.17	0.45
1:B:118:ASN:HD21	1:B:367:LYS:HZ1	1.63	0.45
1:B:246:GLU:N	1:B:250:HIS:HD2	2.14	0.45
1:A:179:ASN:HB2	2:A:1827:HOH:O	2.16	0.45
1:A:605:ARG:NH1	1:B:791:GLU:OE2	2.49	0.45
1:B:532:ILE:O	1:B:535:GLU:HB2	2.15	0.45
1:B:615:GLU:HA	2:B:1514:HOH:O	2.17	0.45
1:A:463:LYS:HB3	1:A:464:TYR:CD1	2.52	0.44
1:A:617:LYS:HB2	2:A:1872:HOH:O	2.17	0.44
1:B:101:MET:HE1	1:B:371:MET:HE2	1.98	0.44
1:B:586:LEU:HD21	1:B:619:VAL:HG13	1.98	0.44
1:A:764:ARG:HA	1:A:764:ARG:HD3	1.62	0.44
1:B:270:VAL:HG21	1:B:291:LEU:HD22	1.98	0.44
1:B:505:ASP:OD1	1:B:522:TYR:OH	2.21	0.44
1:A:802:ASP:HA	1:A:803:PRO:HD2	1.87	0.44
1:B:698:LEU:O	1:B:702:TRP:HB2	2.18	0.44
1:B:709:TYR:HB3	1:B:831:PHE:CD2	2.52	0.44
1:B:205:ALA:HB2	1:B:365:TYR:CE2	2.51	0.44
1:B:423:VAL:HG11	1:B:450:PHE:CZ	2.53	0.44
1:A:286:PRO:HG3	1:A:777:ARG:NH2	2.31	0.44



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:B:81:ARG:HG2	2:B:1378:HOH:O	2.18	0.44	
1:A:219:ARG:HD2	2:A:1678:HOH:O	2.16	0.44	
1:A:709:TYR:HB3	1:A:831:PHE:CD2	2.53	0.44	
1:A:798:MET:HG2	2:A:1385:HOH:O	2.17	0.44	
1:B:367:LYS:HA	2:B:1557:HOH:O	2.18	0.43	
1:B:669:LYS:HB2	1:B:764:ARG:NH1	2.33	0.43	
1:B:694:GLU:H	1:B:694:GLU:HG2	1.61	0.43	
1:A:530:LEU:HB3	1:A:531:PRO:HD3	2.00	0.43	
1:A:661:ARG:NH2	2:A:1576:HOH:O	2.51	0.43	
1:B:242:ALA:N	1:B:243:PRO:HD2	2.33	0.43	
1:B:519:PRO:HD2	2:B:1374:HOH:O	2.18	0.43	
1:B:531:PRO:HB3	2:B:1584:HOH:O	2.17	0.43	
1:B:4:LYS:CG	2:B:1069:HOH:O	2.66	0.43	
1:B:559:GLU:HG2	1:B:630:VAL:HG12	2.01	0.43	
1:B:200:ARG:O	1:B:200:ARG:HG3	2.19	0.43	
1:B:430:GLY:O	1:B:478:ARG:HB2	2.19	0.43	
1:A:241:LEU:O	1:A:245:MET:HG3	2.18	0.43	
1:B:205:ALA:HB2	1:B:365:TYR:CD2	2.53	0.43	
1:B:260:VAL:HG11	1:B:295:LEU:HB2	2.00	0.43	
1:B:442:ARG:HA	1:B:442:ARG:HD2	1.59	0.43	
1:B:687:ALA:HB3	1:B:701:LEU:HD13	2.00	0.43	
1:A:246:GLU:N	1:A:250:HIS:HD2	2.08	0.43	
1:A:451:THR:C	1:A:453:ARG:H	2.22	0.43	
1:B:328:ARG:NH1	1:B:796:ARG:HD2	2.34	0.43	
1:B:463:LYS:HB3	1:B:464:TYR:CD1	2.53	0.43	
1:B:678:ASP:OD1	1:B:823:LYS:HE2	2.18	0.43	
1:A:90:ALA:HB1	1:A:114:PRO:HD3	2.00	0.43	
1:A:233:ASN:N	1:A:233:ASN:ND2	2.66	0.43	
1:A:761:GLY:O	1:A:764:ARG:HB2	2.19	0.43	
1:A:798:MET:O	1:A:801:ARG:HG3	2.18	0.43	
1:B:40:ARG:HD3	2:B:1825:HOH:O	2.18	0.43	
1:A:438:THR:HB	1:A:556:GLU:CG	2.49	0.42	
1:A:329:ARG:HB3	1:A:335:HIS:ND1	2.34	0.42	
1:B:6:LEU:C	1:B:8:LEU:N	2.73	0.42	
1:A:233:ASN:HD22	1:A:233:ASN:H	1.65	0.42	
1:B:464:TYR:CD1	1:B:464:TYR:N	2.87	0.42	
1:B:809:ARG:HD3	2:B:1189:HOH:O	2.20	0.42	
1:A:612:VAL:CG1	1:B:323:ARG:HH22	2.33	0.42	
1:B:223:ILE:HG12	1:B:355:THR:CG2	2.49	0.42	
1:B:559:GLU:CG	1:B:630:VAL:HG11	2.49	0.42	
1:B:617:LYS:HB3	2:B:1908:HOH:O	2.19	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:103:THR:HA	2:A:1132:HOH:O	2.18	0.42
1:A:169:TYR:CE1	1:A:199:GLN:HG2	2.55	0.42
1:A:797:ALA:HA	1:A:801:ARG:HD3	2.01	0.42
1:A:381:GLU:CD	1:A:638:ARG:HH11	2.23	0.42
1:B:410:LYS:HD2	1:B:603:LEU:HB3	2.02	0.42
1:A:205:ALA:HB2	1:A:365:TYR:CE2	2.54	0.42
1:B:107:LYS:HD3	2:B:1001:HOH:O	2.18	0.42
1:B:540:GLU:O	1:B:540:GLU:HG3	2.19	0.42
1:B:770:VAL:O	1:B:774:VAL:HG23	2.20	0.42
1:A:190:MET:HE1	1:A:224:ILE:HD13	2.01	0.42
1:A:674:ASP:O	1:A:678:ASP:HB2	2.20	0.42
1:B:655:ILE:HD13	1:B:655:ILE:HA	1.87	0.42
1:A:660:ARG:O	1:A:661:ARG:C	2.58	0.42
1:B:-5:ARG:HD3	1:B:-5:ARG:HA	1.65	0.42
1:B:39:LEU:HD23	1:B:148:PHE:CE1	2.53	0.42
1:A:561:ARG:O	1:A:561:ARG:HG3	2.19	0.41
1:B:222:LEU:O	1:B:355:THR:HG22	2.20	0.41
1:B:223:ILE:HG23	1:B:352:THR:HG23	2.02	0.41
1:A:451:THR:C	1:A:453:ARG:N	2.74	0.41
1:A:660:ARG:NH1	2:A:1929:HOH:O	2.51	0.41
1:B:133:TYR:CZ	1:B:137:ARG:HD3	2.55	0.41
1:B:453:ARG:HG3	1:B:453:ARG:HH11	1.84	0.41
1:A:796:ARG:HG2	2:A:1785:HOH:O	2.19	0.41
1:B:21:ALA:HB2	1:B:88:MET:HG3	2.03	0.41
1:A:202:HIS:O	1:A:365:TYR:HA	2.21	0.41
1:B:116:TYR:HD1	1:B:151:LEU:CD1	2.31	0.41
1:B:424:ALA:HB2	1:B:455:ILE:HD11	2.01	0.41
1:B:802:ASP:HA	1:B:803:PRO:HD2	1.95	0.41
1:B:6:LEU:C	1:B:8:LEU:H	2.24	0.41
1:B:381:GLU:OE2	1:B:638:ARG:HD2	2.20	0.41
1:B:507:ARG:CG	1:B:507:ARG:NH1	2.75	0.41
1:B:754:LEU:HD13	1:B:763:MET:SD	2.61	0.41
1:A:247:LYS:C	1:A:249:VAL:H	2.23	0.41
1:B:143:GLY:O	1:B:147:ARG:HB2	2.20	0.41
1:A:796:ARG:HD3	2:A:1885:HOH:O	2.21	0.41
1:A:268:GLU:HA	1:A:271:GLU:HB2	2.03	0.41
1:A:381:GLU:OE2	1:A:638:ARG:HD2	2.21	0.41
1:B:152:GLN:HG2	2:B:1365:HOH:O	2.21	0.41
1:B:552:VAL:HG23	1:B:571:SER:HB2	2.03	0.41
1:B:556:GLU:HG2	2:B:1862:HOH:O	2.21	0.41
1:A:242:ALA:N	1:A:243:PRO:HD2	2.36	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:771:LEU:HD23	1:B:771:LEU:HA	1.84	0.40
1:A:801:ARG:NE	1:A:802:ASP:H	2.20	0.40
1:B:186:LEU:HD22	1:B:354:ALA:HB1	2.03	0.40
1:B:326:ILE:HG13	1:B:795:LEU:HD13	2.04	0.40
1:B:653:LYS:HE3	2:B:1235:HOH:O	2.21	0.40
1:A:245:MET:CE	1:A:270:VAL:CG2	2.98	0.40
1:B:325:LEU:HD13	1:B:328:ARG:NH2	2.36	0.40
1:B:397:MET:HE2	2:B:1413:HOH:O	2.21	0.40
1:B:514:ASP:HB3	1:B:517:GLU:HB2	2.03	0.40
1:A:283:ALA:O	1:A:284:ASN:CB	2.68	0.40
1:B:551:TYR:HD1	1:B:579:GLU:HB3	1.86	0.40
1:B:785:GLU:HG3	2:B:1130:HOH:O	2.20	0.40
1:A:101:MET:CE	1:A:371:MET:CE	2.99	0.40
1:A:317:VAL:HG12	1:A:324:VAL:HA	2.04	0.40
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.96	0.40
1:A:702:TRP:CD1	1:A:714:THR:HG23	2.57	0.40
1:B:672:ALA:HB2	1:B:767:GLU:HG2	2.03	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	Perc	entiles
1	А	835/922~(91%)	765 (92%)	57 (7%)	13~(2%)	9	31
1	В	834/922~(90%)	758 (91%)	60 (7%)	16 (2%)	8	26
All	All	1669/1844~(90%)	1523 (91%)	117 (7%)	29 (2%)	9	29

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
1	А	264	GLU	
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	<i>J</i>	1	1 0
Mol	Chain	Res	Type
1	A	714	THR
1	А	715	ALA
1	А	716	ASP
1	В	695	ASP
1	В	734	GLU
1	В	760	GLU
1	А	735	LEU
1	В	229	ASP
1	В	693	ALA
1	А	-5	ARG
1	А	452	LYS
1	В	3	SER
1	В	111	CYS
1	В	717	SER
1	В	758	ALA
1	В	799	ALA
1	В	800	GLN
1	А	107	LYS
1	А	574	GLN
1	А	801	ARG
1	А	802	ASP
1	А	690	GLU
1	А	694	GLU
1	В	311	ASP
1	В	802	ASP
1	В	-4	GLY
1	В	694	GLU
1	В	324	VAL

Continued from previous page...

#### 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	А	696/755~(92%)	577~(83%)	119~(17%)	2 6
1	В	697/755~(92%)	572 (82%)	125 (18%)	2 5
All	All	1393/1510~(92%)	1149 (82%)	244 (18%)	2 6



Mol	Chain	Res	Type
1	А	-15	ASP
1	А	-5	ARG
1	А	-3	SER
1	А	0	ASP
1	А	3	SER
1	А	4	LYS
1	А	5	LEU
1	А	7	ARG
1	А	12	ARG
1	А	15	LYS
1	А	19	LYS
1	А	29	ASP
1	А	35	THR
1	А	40	ARG
1	A	43	THR
1	А	48	ARG
1	A	53	GLN
1	А	78	LEU
1	А	107	LYS
1	А	111	CYS
1	А	136	LYS
1	А	152	GLN
1	А	155	VAL
1	А	193	SER
1	А	210	VAL
1	А	219	ARG
1	А	222	LEU
1	А	225	SER
1	А	232	SER
1	А	233	ASN
1	А	246	GLU
1	А	256	ARG
1	А	259	THR
1	А	262	VAL
1	A	264	GLU
1	А	265	LYS
1	А	271	GLU
1	А	276	ILE
1	А	277	ASP
1	А	296	LYS
1	A	300	LEU
1	A	305	LYS

All (244) residues with a non-rotameric sidechain are listed below:



$\mathbf{Mol}$	Chain	Res	Type
1	А	310	ARG
1	A	316	ILE
1	А	320	PHE
1	A	326	ILE
1	А	328	ARG
1	А	329	ARG
1	A	347	LYS
1	А	359	GLN
1	A	371	MET
1	А	384	GLU
1	А	387	LYS
1	A	396	ASN
1	А	401	ARG
1	А	402	GLU
1	А	405	SER
1	А	413	GLU
1	A	417	ILE
1	А	434	LEU
1	A	438	THR
1	А	442	ARG
1	А	443	SER
1	A	444	GLU
1	А	449	GLN
1	А	452	LYS
1	А	453	ARG
1	А	454	ARG
1	А	460	LEU
1	А	463	LYS
1	А	478	ARG
1	А	485	THR
1	А	490	ARG
1	А	534	LYS
1	А	538	SER
1	А	539	LYS
1	А	542	LYS
1	А	546	GLU
1	А	555	THR
1	А	561	ARG
1	А	592	ARG
1	А	593	ARG
1	А	599	LEU
1	А	600	GLU



Mol	Chain	Res	Type
1	А	601	THR
1	А	603	LEU
1	А	605	ARG
1	А	615	GLU
1	А	618	MET
1	А	632	GLN
1	А	641	VAL
1	А	678	ASP
1	А	690	GLU
1	А	694	GLU
1	А	695	ASP
1	А	698	LEU
1	А	702	TRP
1	А	703	THR
1	А	716	ASP
1	А	735	LEU
1	А	737	GLU
1	А	740	LEU
1	А	741	LYS
1	А	744	GLU
1	А	750	ARG
1	А	778	LYS
1	А	780	ARG
1	А	781	GLU
1	А	793	ILE
1	А	795	LEU
1	А	798	MET
1	А	800	GLN
1	А	801	ARG
1	А	809	ARG
1	A	810	GLU
1	A	818	MET
1	A	822	MET
1	A	826	SER
1	A	827	VAL
1	B	-14	SER
1	В	-5	ARG
1	В	3	SER
1	В	4	LYS
1	В	7	ARG
1	В	8	LEU
1	В	12	ARG



Mol	Chain	Res	Type
1	В	18	LYS
1	В	31	VAL
1	В	35	THR
1	В	40	ARG
1	В	48	ARG
1	В	50	LEU
1	В	52	ASP
1	В	53	GLN
1	В	54	LYS
1	В	55	ASN
1	В	107	LYS
1	В	108	THR
1	В	130	VAL
1	В	152	GLN
1	В	155	VAL
1	В	210	VAL
1	B	212	SER
1	В	219	ARG
1	В	225	SER
1	В	229	ASP
1	В	232	SER
1	В	233	ASN
1	В	240	ARG
1	В	256	ARG
1	В	257	LYS
1	В	258	ARG
1	В	259	THR
1	В	265	LYS
1	В	276	ILE
1	B	284	ASN
1	B	289	SER
1	B	305	LYS
1	B	310	ARG
1	B	311	ASP
1	B	319	GLU
1	B	320	PHE
1	B	323	ARG
	B	326	
1	B	328	ARG
	B	329	ARG
1	B	347	LYS
1	В	351	GLN



Mol	Chain	Res	Type
1	В	355	THR
1	В	359	GLN
1	В	371	MET
1	В	372	THR
1	В	384	GLU
1	В	410	LYS
1	В	411	THR
1	В	413	GLU
1	В	421	ASP
1	В	425	GLU
1	В	429	LYS
1	В	433	VAL
1	В	434	LEU
1	В	438	THR
1	В	442	ARG
1	В	444	GLU
1	В	447	SER
1	В	449	GLN
1	В	453	ARG
1	В	454	ARG
1	В	460	LEU
1	В	478	ARG
1	В	490	ARG
1	В	493	ASP
1	В	507	ARG
1	В	510	GLU
1	В	517	GLU
1	В	534	LYS
1	В	536	GLU
1	В	538	SER
1	В	539	LYS
1	В	540	GLU
1	В	546	GLU
1	В	555	THR
1	В	566	GLN
1	В	573	ARG
1	В	599	LEU
1	В	600	GLU
1	В	601	THR
1	В	605	ARG
1	В	617	LYS
1	В	618	MET



Mol	Chain	Res	Type
1	В	621	ARG
1	В	624	LYS
1	В	629	GLN
1	В	636	GLU
1	В	663	LEU
1	В	669	LYS
1	В	671	GLN
1	В	683	TYR
1	В	688	THR
1	В	694	GLU
1	В	698	LEU
1	В	702	TRP
1	В	705	LEU
1	В	713	ILE
1	В	717	SER
1	В	718	LEU
1	В	737	GLU
1	В	740	LEU
1	В	750	ARG
1	В	754	LEU
1	В	755	GLU
1	В	756	GLU
1	В	760	GLU
1	В	764	ARG
1	В	778	LYS
1	В	796	ARG
1	В	798	MET
1	В	800	GLN
1	В	801	ARG
1	В	810	GLU
1	В	814	MET
1	В	822	MET
1	В	827	VAL
1	В	835	VAL

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

Mol	Chain	Res	Type
1	А	118	ASN
1	А	146	HIS
1	А	203	HIS
1	А	233	ASN



	J	1	1 5
Mol	Chain	Res	Type
1	A	250	HIS
1	А	284	ASN
1	А	293	ASN
1	А	359	GLN
1	А	396	ASN
1	А	506	GLN
1	А	558	HIS
1	А	632	GLN
1	А	649	ASN
1	В	53	GLN
1	В	118	ASN
1	В	146	HIS
1	В	250	HIS
1	В	284	ASN
1	В	293	ASN
1	В	359	GLN
1	В	396	ASN
1	В	461	ASN
1	В	558	HIS
1	В	649	ASN
1	В	671	GLN
1	В	765	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

