



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:53 am BST

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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
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) : 2.11

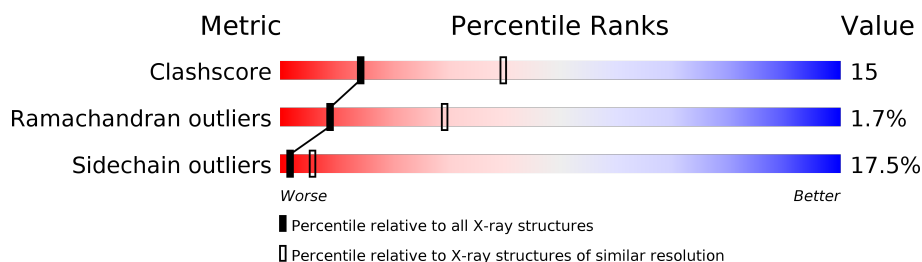
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	922	
1	B	922	

2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6639	4157	1169	1288	25			
1	B	838	Total	C	N	O	S	0	0	0
			6640	4157	1171	1287	25			

There are 62 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	475	Total O 475 475	0	0

Continued on next page...

Continued from previous page...

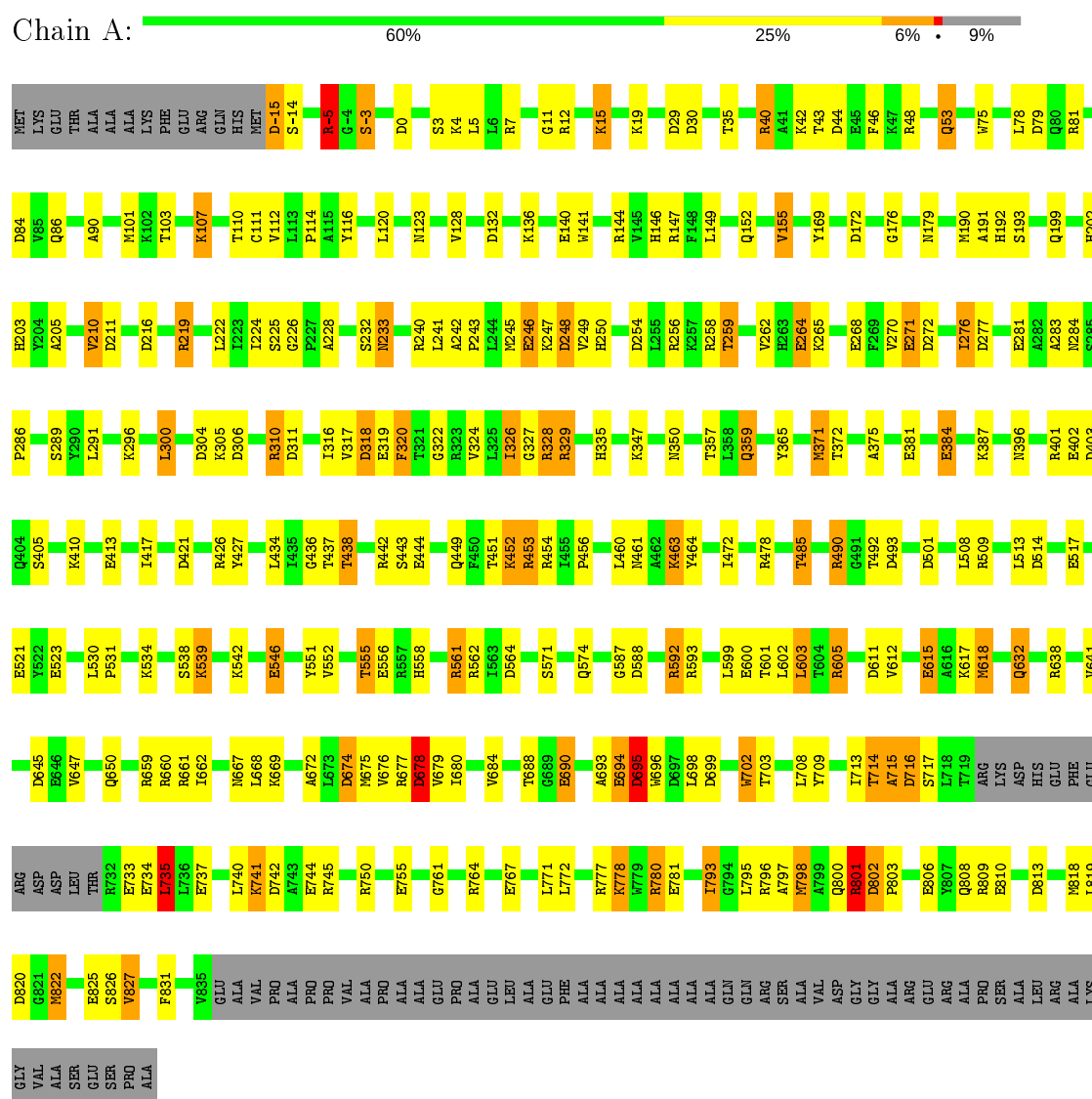
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	455	Total	O	0	0
			455	455		

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 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



• Molecule 1: PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT



U835	A758	D678	E579	R490	E384	Y290	R200	U85	MET
GLU	G759	Y683	L586	D493	V391	L291	R200	P64	LYS
ALA	E760	V684	L586	D501	V391	L295	A205	L78	THR
VAL	M763	D685	R592	D501	M397	E299	V210	D79	ALA
PRO	R764	G686	R593	D505	K410	R303	D211	Q80	ALA
ALA	E767	A687	L599	Q506	T411	D304	S212	R81	LYS
PRO	R768	T688	E600	R507	E412	K305	D216	M88	PHE
VAL	M769	A693	T601	E510	E413	V309	R219	M101	GLU
ALA	M770	D695	L602	E510	E413	R310	R219	M101	ARG
ALA	L771	W696	T604	R511	D421	D311	R219	M101	GLN
ALA	W774	W697	R605	D514	D422	D311	L222	K107	HIS
GLU	W775	L698	L608	E517	V423	D318	L223	T108	MET
PRO	D776	D699	P609	T518	A424	E319	I224	K107	D-15
ALA	R777	A700	P609	P519	E425	F320	S225	T108	S-14
GLU	K778	L701	D610	E520	R426	G321	G226	G111	P-13
LEU	W779	W702	E615	E521	K429	G322	P227	V112	D-12
ALA	R780	L705	A616	Y522	Q430	R323	A228	Y116	R-5
GLU	W781	W709	K617	E523	V433	V324	D229	L117	G-4
PHE	W782	W709	M618	E523	V433	L325	S232	N118	L2
ALA	W785	W709	V619	H527	I434	I326	N233	T129	S3
ALA	W788	W713	T714	S528	I435	G327	K234	V130	K4
ALA	W791	W715	T714	E529	G436	R328	Y235	Y133	L5
ALA	W792	W716	T714	L530	T437	R329	R240	Y133	L6
ALA	W793	W717	K624	P531	T438	R329	R240	K136	R7
ALA	W794	W718	K624	I532	S439	Q336	L241	R137	L8
GLN	W795	L718	Q629	V533	V440	Q336	A242	R137	R12
GLN	L795	W719	V630	K534	P441	K341	P243	W141	K15
ARG	R796	ARG	E636	E535	R442	E342	E246	W142	K18
SER	A797	LYS	V637	E536	S443	E345	R247	G143	K18
ALA	M798	ASP	E637	A537	E444	I346	D248	R144	A21
VAL	A799	HIS	K638	S538	E444	K347	V249	V145	V24
ASP	Q800	GLU	K639	K539	S447	R448	H250	H146	D30
GLY	R801	PHE	E540	E540	Q449	E349	Y251	R147	V31
GLY	D802	GLU	E540	E540	Q449	E349	Y251	F148	T35
ALA	P803	ARG	M643	E543	P450	R350	D254	D163	D86
ARG	E806	ASP	N649	E543	P450	Q351	D254	D163	L39
GLU	Y807	ASP	Q650	E546	R453	T352	L285	R166	R40
ALA	Y807	LEU	R652	E546	R454	T352	R256	R166	A41
ALA	Q808	THR	R653	Y551	I455	A354	K257	M178	K42
PRO	R809	ARG	W654	V552	P456	T355	R258	M179	T43
SER	E810	ARG	L655	V552	H457	I356	T259	D184	D44
ALA	M814	E733	R659	T555	I460	T357	V260	Y185	R48
LEU	W734	L735	R660	E556	I460	T357	V260	L186	L50
ALA	W736	L735	R660	E556	I460	T357	V260	A191	A51
ALA	W737	E737	R661	H558	K463	Q359	K265	D195	Q53
LYS	G821	L740	L662	E559	Y464	L364	V270	D196	K54
GLY	R822	W741	L663	D564	E468	Y365	L276		
VAL	R823	D742	K669	Q566	Y464	D366	D277		
ALA	E824	W742	D670	Q566	I472	K367	N278		
SER	E825	R750	Q671	Q566	I472	M371	E281		
GLU	S826	W750	A672	Q566	R478	T372	E281		
SER	W827	L754	L673	Q566	M486	A375	N284		
PRO	F831	E755	D674	Q566	M486	A375	N284		
ALA	N832	W757	R677	Q566	G489	E381	S289		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	206.20 Å 206.20 Å 295.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.4 (8.00-2.80)	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

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	0.59	0/6743	0.87	26/9116 (0.3%)
1	B	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	A	0	1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	PHE	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	6639	0	6576	197	0
1	B	6640	0	6585	220	0
2	A	475	0	0	57	0
2	B	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 distance (Å)	Clash 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:HH11	1:A:328:ARG:HG3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HH11	1:B:507:ARG:CG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:N	1:A:801:ARG:HE	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:546:GLU:HG3	2:A:1763:HOH:O	1.95	0.65
1:A:326:ILE:HD13	1:B:608:LEU:HD12	1.79	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:HG22	1:A:688:THR:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:VAL:O	1:B:444:GLU:HG2	2.03	0.59
1:B:453:ARG:CG	1:B:453:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:N	1:A:233:ASN:HD22	2.04	0.54
1:A:101:MET:HE3	1:A:371:MET:HE2	1.88	0.54
1:A:612:VAL:HG13	1:B:323:ARG: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:NH1	1:A:328:ARG:HG3	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:NE2	1:A:359:GLN:H	1.89	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:LYS:HE2	2:A:1860:HOH:O	2.10	0.51
1:A:602:LEU:HD11	1:B:791:GLU:O	2.11	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:CD	1:A:53:GLN:H	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:NH1	1:A:328:ARG:CG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:472:ILE:HG13	1:B:489:GLY:HA3	1.97	0.47
1:B:2:LEU:C	1:B:4:LYS:H	2.18	0.47
1:B:764:ARG:HA	1:B:764:ARG:HD3	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:HA	1:B:546:GLU:OE2	2.15	0.47
1:A:509:ARG:HD2	2:A:1828:HOH:O	2.14	0.47
1:A:310:ARG:HE	1:A:310:ARG:HA	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:463:LYS:HE2	2:A:1768:HOH:O	2.14	0.46
1:A:426:ARG:HD3	1:A:551:TYR:CD2	2.50	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:233:ASN:H	1:A:233:ASN:ND2	2.14	0.46
1:A:-5:ARG:HD3	1:A:-5:ARG:HA	1.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HA	1:B:323:ARG:HD2	1.73	0.45
1:B:276:ILE:HG13	1:B:281:GLU:OE2	2.16	0.45
1:B:39:LEU:O	1:B:40:ARG:CB	2.64	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:H	1:B:444:GLU:HG2	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:N	1:A:359:GLN:HE21	1.89	0.45
1:A:546:GLU:HB3	2:A:1726:HOH:O	2.17	0.45
1:B:246:GLU:N	1:B:250:HIS:HD2	2.14	0.45
1:B:118:ASN:HD21	1:B:367:LYS:HZ1	1.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:798:MET:HG2	2:A:1385:HOH:O	2.17	0.44
1:A:709:TYR:HB3	1:A:831:PHE:CD2	2.53	0.44
1:B:367:LYS:HA	2:B:1557:HOH:O	2.18	0.43
1:B:694:GLU:H	1:B:694:GLU:HG2	1.61	0.43
1:B:669:LYS:HB2	1:B:764:ARG:NH1	2.33	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:HD2	1:B:442:ARG:HA	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:ND2	1:A:233:ASN:N	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:H	1:A:233:ASN:HD22	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:B:223:ILE:HG12	1:B:355:THR:CG2	2.49	0.42
1:A:612:VAL:CG1	1:B:323:ARG:HH22	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HG3	1:B:540:GLU:O	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:HA	1:B:655:ILE:HD13	1.87	0.42
1:A:660:ARG:O	1:A:661:ARG:C	2.58	0.42
1:B:39:LEU:HD23	1:B:148:PHE:CE1	2.53	0.42
1:B:-5:ARG:HD3	1:B:-5:ARG:HA	1.65	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:381:GLU:OE2	1:B:638:ARG:HD2	2.20	0.41
1:B:507:ARG:NH1	1:B:507:ARG:CG	2.75	0.41
1:B:6:LEU:C	1:B:8:LEU:H	2.24	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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:326:ILE:HG13	1:B:795:LEU:HD13	2.04	0.40
1:B:186:LEU:HD22	1:B:354:ALA:HB1	2.03	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:HA	1:A:603:LEU:HD12	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

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	835/922 (91%)	765 (92%)	57 (7%)	13 (2%)	9	31
1	B	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	A	264	GLU

Continued on next page...

Continued from previous page...

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

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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	118	ASN
1	A	146	HIS
1	A	203	HIS
1	A	233	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250	HIS
1	A	284	ASN
1	A	293	ASN
1	A	359	GLN
1	A	396	ASN
1	A	506	GLN
1	A	558	HIS
1	A	632	GLN
1	A	649	ASN
1	B	53	GLN
1	B	118	ASN
1	B	146	HIS
1	B	250	HIS
1	B	284	ASN
1	B	293	ASN
1	B	359	GLN
1	B	396	ASN
1	B	461	ASN
1	B	558	HIS
1	B	649	ASN
1	B	671	GLN
1	B	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.