



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:01 am BST

PDB ID : 1NKT  
Title : CRYSTAL STRUCTURE OF THE SECA PROTEIN TRANSLOCATION  
ATPASE FROM MYCOBACTERIUM TUBERCULOSIS COMPLEX WITH  
ADPBS  
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Consortium (TBSGC)  
Deposited on : 2003-01-03  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
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

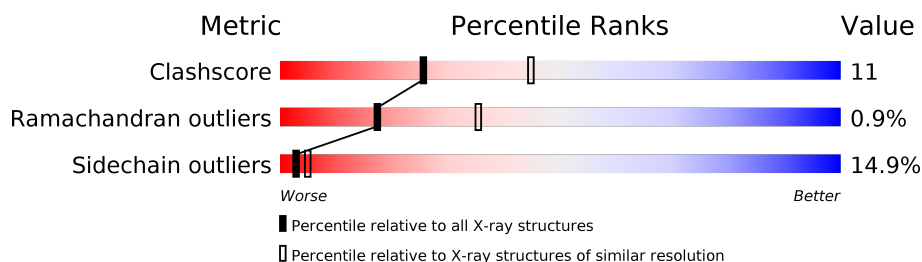
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 4 unique types of molecules in this entry. The entry contains 13862 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	836	Total	C	N	O	S	0	0	0
			6630	4151	1169	1285	25			
1	B	836	Total	C	N	O	S	0	0	0
			6630	4151	1169	1285	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

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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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

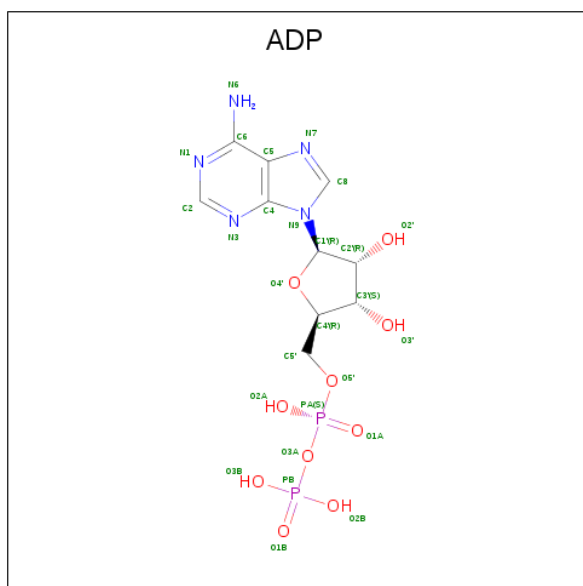
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

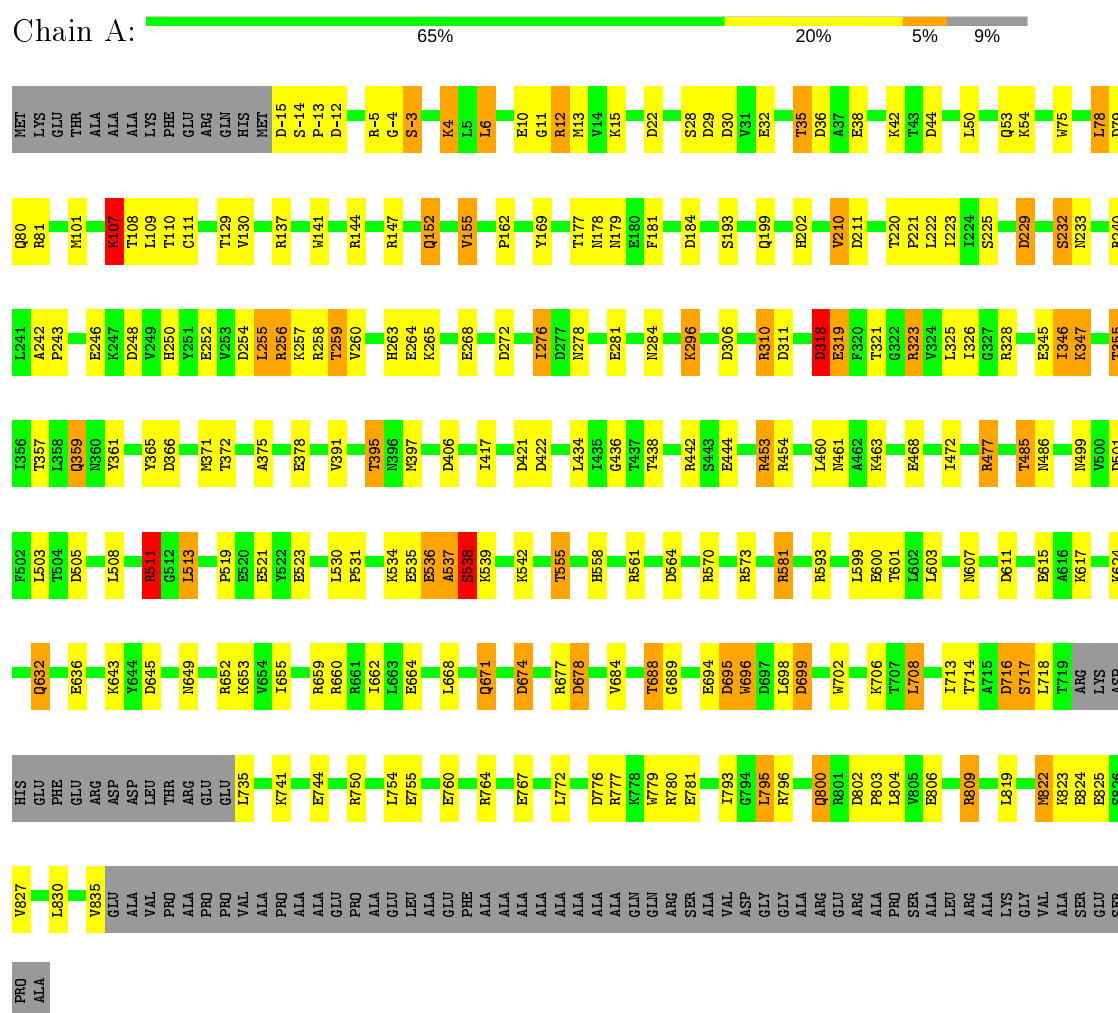
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	246	Total O 246 246	0	0
4	B	300	Total O 300 300	0	0

### 3 Residue-property plots [i](#)

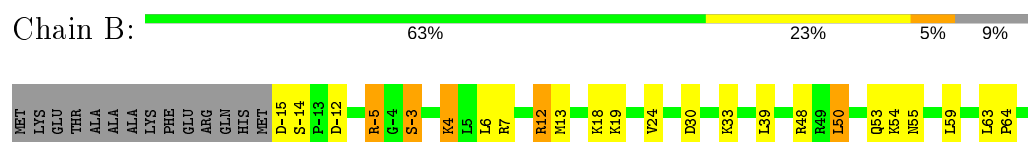
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



VAL	D699	D610	R477	A348	I223	D84
ASP	A700	D611	R478	E349	I224	M101
GLY	W701	V612		N350	S225	
ALA	W702	P613	T485	T355	A228	K107
ARG	T703	E615	N466	I356	D229	T108
ARG	L708	A616	T482	T357	G230	L109
GLU		K617	D493	L358	N233	T110
ARG	T714	M618		Q359		G111
ALA	A715		D501	D366	R240	V112
PRQ	D716	K624	R507	K367	A241	L113
SER	S717	Q632	R511	M371	A242	N118
LEU	L718	Q633		T372	P243	
ARG	T719	R638	E520	A375	E246	T129
ALA	ARG	K639	E523	E381	V249	V130
ALA	LYS	K643	E529	E394	H250	
LYS	ASP	E646	L530	K387	D254	R137
VAL	HIS	N649	I532		K257	G143
ALA	GLU		V633	T395	R258	R144
GLU	PHE	R652	K534	K396	T259	V145
GLU	ARG	K653	E535	M397	E264	H146
ASP	ASP	R659	E536	M399	E268	R147
LEU	LEU	R660	A537	D406	Q152	F148
THR	THR	R661	S538	E413	V153	
ARG	ARG	E666	K539	E417	G154	
GLU	GLU	M667	E540	I417	V155	
GLU	GLU	L668	A541			
VAL	VAL	R669	K542		R165	
ALA	R750	D670	E543	N284	D172	
ALA	L754	Q671	T555	R303		
ALA	E755	A672	H558	D304	N178	
GLU		D674	D564	K305	N179	
PRQ	G759	M675		R310	D184	
ALA		V676	R570	D311		
ALA	E767	R677		D318	R187	
LEU		I680	R573	E319		
ALA	D776	T681		F320	A191	
ALA	R777		R593		H192	
GLU		V684		R323		
PHE	R780	D685	A597	I326	D208	
ALA	E785	G686	A598	G327	E209	
ALA		A687	L599	R329	V210	
ALA	Y788	T688	E600			
ALA		G689	T601	E342	R219	
ALA	R796	E690	L602	E345	T220	
ALA		B694	L603	R329	P221	
ALA	A797		T604		L222	
GLN	M798	E694				
GLN	A799	D695	R605			
ARG	Q800	D696	L608			
SER	R801	D697	P609			
ALA	D802	L698				

## 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, $\alpha$ , $\beta$ , $\gamma$	206.05Å 206.05Å 292.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (95.35-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.213 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.66	2/6734 (0.0%)	0.92	27/9102 (0.3%)
1	B	0.68	1/6734 (0.0%)	0.92	29/9102 (0.3%)
All	All	0.67	3/13468 (0.0%)	0.92	56/18204 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ARG	C-N	6.67	1.45	1.33
1	B	511	ARG	NE-CZ	6.06	1.41	1.33
1	A	513	LEU	CB-CG	5.59	1.68	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	318	ASP	CB-CG-OD2	7.41	124.96	118.30
1	B	79	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	505	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	84	ASP	CB-CG-OD2	6.83	124.44	118.30
1	B	144	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	570	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	184	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	366	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	422	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	155	VAL	CB-CA-C	-6.33	99.37	111.40
1	A	210	VAL	CB-CA-C	-6.32	99.39	111.40
1	B	486	ASN	C-N-CA	-6.31	105.92	121.70
1	A	36	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	318	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	44	ASP	CB-CG-OD2	6.05	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	674	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	155	VAL	CB-CA-C	-5.93	100.13	111.40
1	B	277	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	208	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	813	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	311	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	216	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	678	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	802	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	29	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	406	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	699	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	107	LYS	CD-CE-NZ	5.65	124.70	111.70
1	A	699	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	406	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	-15	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	184	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	610	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	311	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	211	ASP	CB-CG-OD2	5.47	123.23	118.30
1	B	254	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	172	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	30	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	-12	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	501	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	248	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	695	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	674	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	366	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	306	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	434	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	30	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	493	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	144	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	187	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	645	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	22	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	820	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	229	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	6630	0	6581	136	0
1	B	6630	0	6581	151	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	246	0	0	35	0
4	B	300	0	0	42	0
All	All	13862	0	13186	282	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 11.

All (282) 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:11:GLY:HA2	4:A:1387:HOH:O	1.53	1.08
1:A:809:ARG:HB3	1:A:809:ARG:HH11	1.26	1.00
1:A:107:LYS:HD3	4:A:1370:HOH:O	1.62	0.98
1:A:107:LYS:CD	4:A:1370:HOH:O	2.14	0.95
1:A:660:ARG:HG2	4:A:1349:HOH:O	1.66	0.93
1:B:101:MET:HE1	1:B:110:THR:HG21	1.47	0.93
1:B:147:ARG:HD2	4:B:1211:HOH:O	1.66	0.93
1:A:359:GLN:H	1:A:359:GLN:HE21	1.15	0.91
1:A:35:THR:HG22	1:A:38:GLU:H	1.32	0.91
1:A:809:ARG:CB	1:A:809:ARG:HH11	1.85	0.89
1:A:777:ARG:NH2	1:A:825:GLU:OE1	2.06	0.88
1:B:454:ARG:HG3	1:B:454:ARG:O	1.72	0.88
1:B:660:ARG:HG3	4:B:1355:HOH:O	1.74	0.87
1:A:461:ASN:HA	1:A:485:THR:HG23	1.56	0.86
1:A:534:LYS:O	1:A:538:SER:HB3	1.75	0.86
1:B:233:ASN:H	1:B:233:ASN:HD22	1.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:GLU:HG2	4:A:1502:HOH:O	1.75	0.85
1:B:6:LEU:HD12	4:B:1433:HOH:O	1.77	0.85
1:B:666:GLU:HG3	4:B:1491:HOH:O	1.75	0.84
1:B:611:ASP:HB3	4:B:1296:HOH:O	1.77	0.84
1:B:359:GLN:H	1:B:359:GLN:HE21	1.20	0.83
1:B:346:ILE:HB	4:B:1180:HOH:O	1.80	0.81
1:A:395:THR:CG2	1:A:397:MET:O	2.28	0.81
1:A:643:LYS:HD3	1:A:804:LEU:HD22	1.62	0.80
1:B:780:ARG:HD3	4:B:1519:HOH:O	1.80	0.79
1:B:785:GLU:OE1	4:B:1414:HOH:O	2.00	0.79
1:B:809:ARG:HD3	4:B:1131:HOH:O	1.81	0.79
1:A:511:ARG:NH1	4:A:1210:HOH:O	2.15	0.79
1:B:329:ARG:HD3	4:B:1414:HOH:O	1.81	0.78
1:B:395:THR:HG23	1:B:397:MET:O	1.83	0.77
1:B:461:ASN:HA	1:B:485:THR:HG23	1.65	0.77
1:B:511:ARG:NH2	1:B:529:GLU:OE2	2.18	0.77
1:B:246:GLU:H	1:B:250:HIS:HD2	1.30	0.77
1:B:785:GLU:HG3	4:B:1092:HOH:O	1.85	0.76
1:B:660:ARG:CG	4:B:1355:HOH:O	2.32	0.75
1:A:436:GLY:O	1:A:555:THR:HB	1.86	0.75
1:B:129:THR:HB	4:B:1212:HOH:O	1.87	0.75
1:A:678:ASP:OD1	1:A:823:LYS:HE3	1.87	0.75
1:B:-5:ARG:HD2	4:B:1489:HOH:O	1.87	0.73
1:B:558:HIS:HD2	1:B:564:ASP:OD2	1.73	0.71
1:B:501:ASP:HB3	4:B:1229:HOH:O	1.90	0.71
1:A:660:ARG:CG	4:A:1349:HOH:O	2.33	0.70
1:B:101:MET:CE	1:B:110:THR:HG21	2.22	0.70
1:B:192:HIS:HD2	4:B:1510:HOH:O	1.74	0.69
1:B:454:ARG:HH11	1:B:454:ARG:HB2	1.57	0.69
1:A:80:GLN:HE21	1:A:109:LEU:HD22	1.57	0.69
1:B:698:LEU:HD11	4:B:1295:HOH:O	1.93	0.69
1:B:649:ASN:HD22	1:B:652:ARG:HH21	1.41	0.68
1:B:228:ALA:HB3	4:B:1292:HOH:O	1.94	0.68
1:A:809:ARG:CB	1:A:809:ARG:NH1	2.56	0.67
1:B:246:GLU:H	1:B:250:HIS:CD2	2.11	0.67
1:B:258:ARG:HH11	1:B:258:ARG:HB2	1.58	0.67
1:B:144:ARG:HD2	1:B:523:GLU:OE2	1.95	0.67
1:A:643:LYS:HE2	4:A:1464:HOH:O	1.95	0.66
1:B:674:ASP:OD1	1:B:677:ARG:NH1	2.22	0.66
1:B:346:ILE:HG22	4:B:1494:HOH:O	1.96	0.66
1:A:276:ILE:HG13	1:A:281:GLU:OE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:THR:CG2	1:B:375:ALA:HB2	2.27	0.65
1:A:809:ARG:NE	4:A:1149:HOH:O	2.30	0.65
1:B:436:GLY:O	1:B:555:THR:HB	1.96	0.65
1:B:233:ASN:ND2	1:B:233:ASN:H	1.95	0.64
1:B:357:THR:HB	1:B:359:GLN:NE2	2.13	0.64
1:B:735:LEU:N	4:B:1166:HOH:O	2.30	0.64
1:B:719:THR:HG22	1:B:719:THR:O	1.97	0.63
1:A:581:ARG:HD2	4:A:1298:HOH:O	1.98	0.63
1:A:809:ARG:HD3	4:A:1149:HOH:O	1.98	0.63
1:A:255:LEU:HD12	1:A:256:ARG:HD2	1.81	0.63
1:B:191:ALA:O	1:B:659:ARG:NH2	2.32	0.63
1:B:276:ILE:HG13	1:B:281:GLU:OE2	1.98	0.63
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.63	0.62
1:B:649:ASN:HD22	1:B:652:ARG:NH2	1.97	0.62
1:A:246:GLU:H	1:A:250:HIS:CD2	2.18	0.61
1:A:395:THR:HG22	1:A:397:MET:O	1.98	0.61
1:A:12:ARG:HH11	1:A:12:ARG:CG	2.14	0.61
1:B:534:LYS:O	1:B:538:SER:HB3	2.00	0.61
1:A:246:GLU:H	1:A:250:HIS:HD2	1.49	0.61
1:A:144:ARG:HD2	1:A:523:GLU:OE2	2.01	0.60
1:A:421:ASP:OD1	1:A:453:ARG:NH2	2.34	0.60
1:B:347:LYS:HD3	4:B:1526:HOH:O	2.00	0.60
1:A:223:ILE:HG12	1:A:355:THR:HG23	1.84	0.60
1:B:597:ALA:O	1:B:601:THR:HG23	2.01	0.60
1:B:777:ARG:NH2	1:B:825:GLU:OE1	2.35	0.60
1:A:780:ARG:HD2	4:A:1506:HOH:O	2.02	0.59
1:B:659:ARG:NH1	1:B:776:ASP:OD1	2.33	0.59
1:A:147:ARG:HD2	4:A:1371:HOH:O	2.01	0.59
1:B:350:ASN:HB3	4:B:1254:HOH:O	2.03	0.58
1:B:101:MET:O	1:B:107:LYS:HE2	2.02	0.58
1:A:611:ASP:HB3	4:A:1498:HOH:O	2.04	0.58
1:B:798:MET:HG2	1:B:800:GLN:HB2	1.86	0.58
1:B:804:LEU:O	1:B:808:GLN:HG3	2.03	0.58
1:A:684:VAL:O	1:A:688:THR:HB	2.03	0.57
1:B:395:THR:CG2	1:B:397:MET:O	2.52	0.57
1:B:493:ASP:OD2	1:B:573:ARG:NH1	2.35	0.57
1:A:780:ARG:CD	4:A:1506:HOH:O	2.53	0.57
1:A:535:GLU:O	1:A:537:ALA:O	2.23	0.57
1:A:346:ILE:HG13	4:A:1430:HOH:O	2.04	0.57
1:A:129:THR:HB	4:A:1383:HOH:O	2.05	0.56
1:B:677:ARG:O	1:B:681:THR:OG1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:TYR:HB3	4:B:1334:HOH:O	2.06	0.56
1:B:372:THR:HG21	1:B:375:ALA:HB2	1.88	0.55
1:B:558:HIS:HE1	4:B:1456:HOH:O	1.89	0.55
1:A:809:ARG:CD	4:A:1149:HOH:O	2.51	0.55
1:A:310:ARG:HE	1:A:310:ARG:HA	1.72	0.55
1:B:219:ARG:HD2	4:B:1259:HOH:O	2.06	0.55
1:B:223:ILE:HG12	1:B:355:THR:HG23	1.88	0.55
1:B:461:ASN:OD1	1:B:485:THR:HG21	2.06	0.55
1:B:454:ARG:CB	1:B:454:ARG:HH11	2.19	0.55
1:A:764:ARG:HA	1:A:767:GLU:OE1	2.07	0.55
1:B:-3:SER:HB3	4:B:1375:HOH:O	2.05	0.55
1:A:323:ARG:HE	1:B:615:GLU:HB2	1.72	0.55
1:B:381:GLU:OE2	1:B:638:ARG:HD2	2.08	0.54
1:A:346:ILE:HB	4:A:1430:HOH:O	2.06	0.54
1:A:357:THR:HB	1:A:359:GLN:NE2	2.22	0.54
1:A:107:LYS:CE	4:A:1370:HOH:O	2.54	0.54
1:A:793:ILE:HD12	1:A:796:ARG:CZ	2.37	0.54
1:B:680:ILE:O	1:B:684:VAL:HG23	2.08	0.54
1:A:793:ILE:HD12	1:A:796:ARG:NH1	2.23	0.53
1:B:129:THR:CB	4:B:1212:HOH:O	2.52	0.53
1:B:461:ASN:OD1	1:B:485:THR:CG2	2.56	0.53
1:B:303:ARG:O	1:B:304:ASP:HB2	2.09	0.53
1:A:561:ARG:O	1:A:564:ASP:HB2	2.09	0.53
1:B:671:GLN:H	1:B:671:GLN:HE21	1.58	0.52
1:B:798:MET:HG3	1:B:799:ALA:N	2.24	0.52
1:B:714:THR:O	1:B:717:SER:HB2	2.10	0.52
1:A:325:LEU:HD22	1:A:328:ARG:HH21	1.75	0.52
1:B:600:GLU:HG3	1:B:601:THR:N	2.24	0.52
1:B:63:LEU:HB3	1:B:64:PRO:HD3	1.92	0.52
1:B:767:GLU:HA	1:B:830:LEU:HD21	1.92	0.52
1:A:767:GLU:HA	1:A:830:LEU:HD21	1.92	0.52
1:B:649:ASN:O	1:B:653:LYS:HG2	2.10	0.52
1:A:461:ASN:OD1	1:A:485:THR:HG21	2.10	0.51
1:B:671:GLN:H	1:B:671:GLN:NE2	2.09	0.51
1:A:461:ASN:OD1	1:A:485:THR:CG2	2.58	0.51
1:B:687:ALA:HB3	1:B:701:LEU:HD13	1.91	0.51
1:A:107:LYS:HE3	4:A:1370:HOH:O	2.10	0.51
1:A:177:THR:HG23	4:A:1361:HOH:O	2.10	0.51
1:A:674:ASP:OD1	1:A:677:ARG:NH1	2.40	0.51
1:B:558:HIS:CD2	1:B:564:ASP:OD2	2.59	0.51
1:B:478:ARG:HD3	1:B:543:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:GLU:HA	1:B:532:ILE:HD12	1.93	0.51
1:B:780:ARG:HG2	4:B:1405:HOH:O	2.10	0.50
1:A:372:THR:HG21	1:A:375:ALA:HB2	1.94	0.50
1:B:801:ARG:NH1	1:B:806:GLU:HG3	2.25	0.50
1:A:558:HIS:HD2	1:A:564:ASP:OD2	1.94	0.50
1:B:242:ALA:HB3	1:B:243:PRO:HD3	1.94	0.50
4:A:1299:HOH:O	1:B:310:ARG:HD3	2.10	0.50
1:A:708:LEU:HD12	1:A:827:VAL:HG22	1.94	0.50
1:A:35:THR:HG22	1:A:38:GLU:N	2.14	0.50
1:B:536:GLU:C	1:B:537:ALA:O	2.49	0.50
1:B:107:LYS:HE3	3:B:901:ADP:O1B	2.12	0.50
1:B:639:LYS:O	1:B:643:LYS:HG3	2.12	0.50
1:B:796:ARG:HD2	4:B:1250:HOH:O	2.12	0.50
1:A:607:ASN:ND2	1:B:788:TYR:OH	2.35	0.49
1:A:372:THR:CG2	1:A:375:ALA:HB2	2.42	0.49
1:A:649:ASN:HD22	1:A:652:ARG:HH21	1.59	0.49
1:A:162:PRO:HD2	4:A:1413:HOH:O	2.13	0.49
1:A:714:THR:HB	1:A:717:SER:H	1.78	0.49
1:B:19:LYS:HD3	4:B:1468:HOH:O	2.12	0.49
1:A:793:ILE:HD11	1:A:806:GLU:HB3	1.94	0.49
1:B:801:ARG:HH11	1:B:806:GLU:HG3	1.77	0.48
1:A:242:ALA:N	1:A:243:PRO:HD2	2.29	0.48
1:A:359:GLN:NE2	1:A:359:GLN:H	1.97	0.48
1:A:35:THR:HG23	4:A:1182:HOH:O	2.12	0.48
1:A:310:ARG:HG2	1:B:612:VAL:HG22	1.94	0.48
1:A:819:LEU:HA	1:A:822:MET:HE2	1.95	0.48
1:B:632:GLN:NE2	1:B:632:GLN:HA	2.28	0.48
1:A:101:MET:CE	1:A:110:THR:HG21	2.44	0.48
1:B:118:ASN:HD21	1:B:367:LYS:NZ	2.12	0.48
1:B:687:ALA:CB	1:B:701:LEU:HD13	2.43	0.48
1:B:80:GLN:HE21	1:B:109:LEU:HD22	1.79	0.48
1:B:139:SER:O	1:B:143:GLY:HA3	2.14	0.48
1:B:649:ASN:ND2	1:B:652:ARG:HH21	2.08	0.48
1:B:681:THR:O	1:B:685:ASP:HB2	2.13	0.48
1:A:649:ASN:O	1:A:653:LYS:HG2	2.14	0.48
1:A:713:ILE:HD12	1:A:718:LEU:HD11	1.96	0.48
1:A:558:HIS:HE1	4:A:1421:HOH:O	1.97	0.47
1:B:112:VAL:HG13	1:B:146:HIS:CE1	2.50	0.47
1:B:254:ASP:OD2	1:B:257:LYS:HB2	2.14	0.47
1:A:537:ALA:O	1:A:539:LYS:N	2.46	0.47
1:B:438:THR:HG23	1:B:438:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLN:NE2	1:A:109:LEU:HD22	2.27	0.47
1:A:6:LEU:HD21	1:A:391:VAL:HG22	1.96	0.47
1:B:681:THR:HG23	1:B:736:LEU:HD21	1.96	0.47
1:A:347:LYS:HD2	4:A:1095:HOH:O	2.15	0.47
1:A:35:THR:HB	1:A:38:GLU:OE1	2.14	0.47
1:A:668:LEU:HD22	1:A:671:GLN:HG3	1.96	0.47
1:B:178:ASN:OD1	1:B:358:LEU:HD21	2.15	0.47
1:B:12:ARG:HG2	4:B:1469:HOH:O	2.13	0.47
1:A:659:ARG:HD2	1:A:776:ASP:OD1	2.15	0.46
1:B:147:ARG:CD	4:B:1211:HOH:O	2.42	0.46
1:B:24:VAL:HG22	1:B:64:PRO:HA	1.97	0.46
1:B:78:LEU:HB3	1:B:80:GLN:HG2	1.97	0.46
1:A:141:TRP:O	1:A:144:ARG:HG3	2.15	0.46
1:A:662:ILE:HG21	1:A:772:LEU:HB2	1.97	0.46
1:A:10:GLU:HA	1:A:10:GLU:OE1	2.15	0.46
1:A:809:ARG:HB2	1:A:809:ARG:NH1	2.30	0.46
1:B:530:LEU:HB3	1:B:531:PRO:HD3	1.98	0.46
1:A:477:ARG:HD2	4:A:1290:HOH:O	2.15	0.46
1:A:615:GLU:HG2	4:B:1226:HOH:O	2.14	0.46
1:A:75:TRP:HB2	1:A:81:ARG:HB2	1.98	0.46
1:A:310:ARG:HG2	1:B:612:VAL:CG2	2.46	0.46
1:B:413:GLU:HA	4:B:1331:HOH:O	2.16	0.46
1:A:152:GLN:HE21	1:A:152:GLN:HB3	1.57	0.45
1:A:178:ASN:ND2	4:A:1153:HOH:O	2.44	0.45
1:A:395:THR:HG21	1:A:397:MET:O	2.12	0.45
1:A:15:LYS:HD3	4:A:1310:HOH:O	2.16	0.45
1:B:670:ASP:HB2	1:B:671:GLN:NE2	2.32	0.45
1:B:220:THR:HA	1:B:221:PRO:HD3	1.86	0.45
1:B:672:ALA:HA	1:B:675:MET:HE2	1.98	0.45
1:A:-14:SER:HB3	1:A:-13:PRO:HD2	1.99	0.45
1:A:819:LEU:HD23	1:A:822:MET:CE	2.47	0.45
1:B:661:ARG:HD2	1:B:668:LEU:HD21	1.97	0.45
1:A:536:GLU:C	1:A:537:ALA:O	2.55	0.44
1:A:671:GLN:H	1:A:671:GLN:CD	2.21	0.44
1:B:39:LEU:HD23	1:B:148:PHE:HE1	1.83	0.44
1:B:735:LEU:CA	4:B:1166:HOH:O	2.65	0.44
1:B:137:ARG:HD3	4:B:1222:HOH:O	2.17	0.44
1:A:35:THR:HB	1:A:38:GLU:HB2	1.99	0.44
1:A:42:LYS:HD2	1:A:42:LYS:HA	1.76	0.44
1:B:276:ILE:HG13	1:B:281:GLU:CD	2.37	0.44
1:B:671:GLN:NE2	1:B:671:GLN:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:LEU:HD12	4:B:1241:HOH:O	2.17	0.44
1:A:169:TYR:CZ	1:A:199:GLN:HG2	2.53	0.44
1:A:819:LEU:HD23	1:A:822:MET:HE2	2.00	0.44
1:A:-5:ARG:O	1:A:-3:SER:N	2.51	0.44
1:B:477:ARG:HD3	1:B:540:GLU:HG2	1.98	0.44
1:A:780:ARG:NE	4:A:1506:HOH:O	2.51	0.44
1:B:165:ARG:HD3	1:B:184:ASP:OD1	2.17	0.43
1:A:202:HIS:O	1:A:365:TYR:HA	2.18	0.43
1:A:260:VAL:HG23	1:A:296:LYS:HG2	2.00	0.43
1:A:655:ILE:HG13	1:A:779:TRP:CE3	2.53	0.43
1:B:4:LYS:HE3	1:B:4:LYS:HA	1.99	0.43
1:B:67:PHE:CD1	1:B:113:LEU:HB3	2.53	0.43
1:A:220:THR:HA	1:A:221:PRO:HD3	1.87	0.43
1:B:222:LEU:O	1:B:355:THR:CG2	2.66	0.43
1:A:714:THR:HG22	1:A:716:ASP:H	1.83	0.43
1:A:780:ARG:HD3	4:A:1490:HOH:O	2.19	0.43
1:A:181:PHE:HB3	1:A:361:TYR:OH	2.17	0.43
1:A:328:ARG:HH12	1:A:796:ARG:HE	1.66	0.43
1:A:460:LEU:HD22	1:A:468:GLU:HG2	1.99	0.43
1:A:4:LYS:HA	4:A:1418:HOH:O	2.18	0.43
1:B:284:ASN:HA	4:B:1524:HOH:O	2.19	0.43
1:A:78:LEU:HB3	1:A:80:GLN:HG2	2.00	0.43
1:A:802:ASP:HA	1:A:803:PRO:HD3	1.86	0.43
1:B:608:LEU:HA	1:B:609:PRO:HD3	1.93	0.43
1:B:143:GLY:HA2	1:B:153:VAL:HG21	2.01	0.43
1:B:537:ALA:O	1:B:538:SER:HB3	2.19	0.43
1:B:179:ASN:HB2	4:B:1081:HOH:O	2.19	0.43
1:B:254:ASP:HB3	1:B:259:THR:HG22	2.01	0.43
1:B:612:VAL:HA	1:B:613:PRO:HD3	1.94	0.43
1:B:472:ILE:HG21	1:B:492:THR:HB	2.00	0.42
1:B:50:LEU:HD11	1:B:59:LEU:CD2	2.49	0.42
1:A:328:ARG:HH12	1:A:796:ARG:NE	2.16	0.42
1:A:278:ASN:O	1:A:281:GLU:HG2	2.19	0.42
1:B:246:GLU:HB3	1:B:249:VAL:HB	2.01	0.42
1:A:519:PRO:HD2	4:A:1410:HOH:O	2.18	0.42
1:A:649:ASN:HD22	1:A:652:ARG:NH2	2.17	0.42
1:B:463:LYS:HD2	1:B:463:LYS:HA	1.86	0.42
1:B:646:GLU:OE1	1:B:646:GLU:HA	2.19	0.42
1:A:108:THR:O	1:A:111:CYS:HB3	2.19	0.42
1:A:232:SER:HB3	1:A:346:ILE:HD12	2.02	0.42
1:B:216:ASP:O	1:B:219:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:HD2	1:B:342:GLU:OE1	2.20	0.41
1:B:694:GLU:O	1:B:696:TRP:N	2.53	0.41
1:A:499:ASN:O	1:A:503:LEU:HD12	2.20	0.41
1:A:513:LEU:CD2	1:A:521:GLU:HB3	2.51	0.41
1:A:632:GLN:O	1:A:636:GLU:HG2	2.20	0.41
1:B:55:ASN:HB3	4:B:1271:HOH:O	2.21	0.41
1:B:605:ARG:HE	1:B:605:ARG:HB2	1.80	0.41
1:B:78:LEU:O	1:B:79:ASP:HB2	2.19	0.41
1:B:755:GLU:O	1:B:759:GLY:N	2.53	0.41
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.70	0.41
1:A:318:ASP:C	1:A:318:ASP:OD2	2.59	0.41
1:A:694:GLU:O	1:A:696:TRP:N	2.54	0.41
1:B:-15:ASP:HB3	4:B:1068:HOH:O	2.21	0.41
1:A:254:ASP:HB2	1:A:259:THR:HG22	2.03	0.40
1:A:615:GLU:HG3	1:B:323:ARG:HG3	2.03	0.40
1:B:660:ARG:HG2	4:B:1355:HOH:O	2.09	0.40
1:A:229:ASP:HB3	4:A:1506:HOH:O	2.21	0.40
1:B:818:MET:O	1:B:822:MET:HG3	2.21	0.40
1:A:530:LEU:HB3	1:A:531:PRO:HD3	2.03	0.40
1:A:250:HIS:O	1:A:263:HIS:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	832/922 (90%)	781 (94%)	41 (5%)	10 (1%)	13	27
1	B	832/922 (90%)	784 (94%)	43 (5%)	5 (1%)	25	47
All	All	1664/1844 (90%)	1565 (94%)	84 (5%)	15 (1%)	17	35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	486	ASN
1	A	538	SER
1	A	689	GLY
1	A	695	ASP
1	B	695	ASP
1	A	-4	GLY
1	A	537	ALA
1	A	760	GLU
1	A	800	GLN
1	B	319	GLU
1	A	795	LEU
1	B	689	GLY
1	B	800	GLN
1	B	230	GLY

### 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	697/755 (92%)	592 (85%)	105 (15%)	3	4
1	B	697/755 (92%)	594 (85%)	103 (15%)	3	5
All	All	1394/1510 (92%)	1186 (85%)	208 (15%)	3	5

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-12	ASP
1	A	-3	SER
1	A	4	LYS
1	A	6	LEU
1	A	12	ARG
1	A	13	MET
1	A	28	SER
1	A	32	GLU
1	A	35	THR

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Mol	Chain	Res	Type
1	A	50	LEU
1	A	53	GLN
1	A	54	LYS
1	A	78	LEU
1	A	107	LYS
1	A	130	VAL
1	A	137	ARG
1	A	152	GLN
1	A	155	VAL
1	A	179	ASN
1	A	193	SER
1	A	210	VAL
1	A	222	LEU
1	A	225	SER
1	A	232	SER
1	A	233	ASN
1	A	240	ARG
1	A	252	GLU
1	A	255	LEU
1	A	256	ARG
1	A	257	LYS
1	A	258	ARG
1	A	259	THR
1	A	264	GLU
1	A	265	LYS
1	A	268	GLU
1	A	272	ASP
1	A	276	ILE
1	A	284	ASN
1	A	296	LYS
1	A	310	ARG
1	A	318	ASP
1	A	319	GLU
1	A	321	THR
1	A	323	ARG
1	A	326	ILE
1	A	345	GLU
1	A	346	ILE
1	A	347	LYS
1	A	355	THR
1	A	359	GLN
1	A	371	MET

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Mol	Chain	Res	Type
1	A	378	GLU
1	A	395	THR
1	A	417	ILE
1	A	434	LEU
1	A	438	THR
1	A	442	ARG
1	A	444	GLU
1	A	453	ARG
1	A	454	ARG
1	A	463	LYS
1	A	472	ILE
1	A	477	ARG
1	A	485	THR
1	A	508	LEU
1	A	511	ARG
1	A	536	GLU
1	A	538	SER
1	A	542	LYS
1	A	555	THR
1	A	570	ARG
1	A	573	ARG
1	A	581	ARG
1	A	593	ARG
1	A	599	LEU
1	A	600	GLU
1	A	601	THR
1	A	603	LEU
1	A	617	LYS
1	A	624	LYS
1	A	632	GLN
1	A	664	GLU
1	A	671	GLN
1	A	688	THR
1	A	696	TRP
1	A	698	LEU
1	A	699	ASP
1	A	702	TRP
1	A	706	LYS
1	A	708	LEU
1	A	716	ASP
1	A	717	SER
1	A	735	LEU

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Mol	Chain	Res	Type
1	A	741	LYS
1	A	744	GLU
1	A	750	ARG
1	A	754	LEU
1	A	755	GLU
1	A	781	GLU
1	A	795	LEU
1	A	800	GLN
1	A	809	ARG
1	A	822	MET
1	A	824	GLU
1	A	835	VAL
1	B	-14	SER
1	B	-5	ARG
1	B	-3	SER
1	B	4	LYS
1	B	7	ARG
1	B	12	ARG
1	B	13	MET
1	B	18	LYS
1	B	33	LYS
1	B	48	ARG
1	B	50	LEU
1	B	53	GLN
1	B	54	LYS
1	B	78	LEU
1	B	130	VAL
1	B	137	ARG
1	B	152	GLN
1	B	155	VAL
1	B	195	ASP
1	B	210	VAL
1	B	222	LEU
1	B	225	SER
1	B	229	ASP
1	B	233	ASN
1	B	240	ARG
1	B	258	ARG
1	B	259	THR
1	B	264	GLU
1	B	268	GLU
1	B	276	ILE

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Mol	Chain	Res	Type
1	B	277	ASP
1	B	305	LYS
1	B	318	ASP
1	B	319	GLU
1	B	320	PHE
1	B	326	ILE
1	B	328	ARG
1	B	345	GLU
1	B	347	LYS
1	B	349	GLU
1	B	355	THR
1	B	359	GLN
1	B	371	MET
1	B	384	GLU
1	B	387	LYS
1	B	395	THR
1	B	399	MET
1	B	417	ILE
1	B	425	GLU
1	B	429	LYS
1	B	434	LEU
1	B	438	THR
1	B	441	GLU
1	B	442	ARG
1	B	444	GLU
1	B	452	LYS
1	B	454	ARG
1	B	463	LYS
1	B	472	ILE
1	B	485	THR
1	B	507	ARG
1	B	520	GLU
1	B	535	GLU
1	B	539	LYS
1	B	542	LYS
1	B	555	THR
1	B	573	ARG
1	B	593	ARG
1	B	599	LEU
1	B	600	GLU
1	B	603	LEU
1	B	605	ARG

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Mol	Chain	Res	Type
1	B	617	LYS
1	B	618	MET
1	B	624	LYS
1	B	632	GLN
1	B	633	GLN
1	B	646	GLU
1	B	671	GLN
1	B	681	THR
1	B	688	THR
1	B	690	GLU
1	B	694	GLU
1	B	698	LEU
1	B	699	ASP
1	B	702	TRP
1	B	703	THR
1	B	708	LEU
1	B	716	ASP
1	B	717	SER
1	B	718	LEU
1	B	735	LEU
1	B	737	GLU
1	B	750	ARG
1	B	754	LEU
1	B	780	ARG
1	B	798	MET
1	B	800	GLN
1	B	810	GLU
1	B	823	LYS
1	B	827	VAL
1	B	833	VAL
1	B	835	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	118	ASN
1	A	146	HIS
1	A	152	GLN
1	A	203	HIS
1	A	233	ASN
1	A	250	HIS

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Mol	Chain	Res	Type
1	A	293	ASN
1	A	359	GLN
1	A	396	ASN
1	A	558	HIS
1	A	607	ASN
1	A	649	ASN
1	A	671	GLN
1	B	80	GLN
1	B	118	ASN
1	B	146	HIS
1	B	152	GLN
1	B	192	HIS
1	B	233	ASN
1	B	250	HIS
1	B	293	ASN
1	B	359	GLN
1	B	396	ASN
1	B	558	HIS
1	B	632	GLN
1	B	649	ASN
1	B	671	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	A	900	2	24,29,29	1.34	3 (12%)	29,45,45	1.74	3 (10%)
3	ADP	B	901	2	24,29,29	1.31	3 (12%)	29,45,45	1.69	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	900	2	-	4/12/32/32	0/3/3/3
3	ADP	B	901	2	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	ADP	C2-N3	4.26	1.39	1.32
3	A	900	ADP	C2-N3	4.18	1.38	1.32
3	B	901	ADP	C2-N1	2.99	1.39	1.33
3	A	900	ADP	C2-N1	2.65	1.38	1.33
3	B	901	ADP	PB-O3B	2.36	1.63	1.54
3	A	900	ADP	PB-O3B	2.13	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	ADP	N3-C2-N1	-6.55	118.44	128.68
3	B	901	ADP	N3-C2-N1	-5.50	120.07	128.68
3	B	901	ADP	O3B-PB-O3A	3.48	116.32	104.64
3	A	900	ADP	O3A-PB-O1B	-3.36	92.56	111.19
3	B	901	ADP	O3A-PB-O1B	-3.26	93.11	111.19
3	B	901	ADP	PA-O3A-PB	-2.39	124.61	132.83
3	A	900	ADP	O3B-PB-O3A	2.24	112.16	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

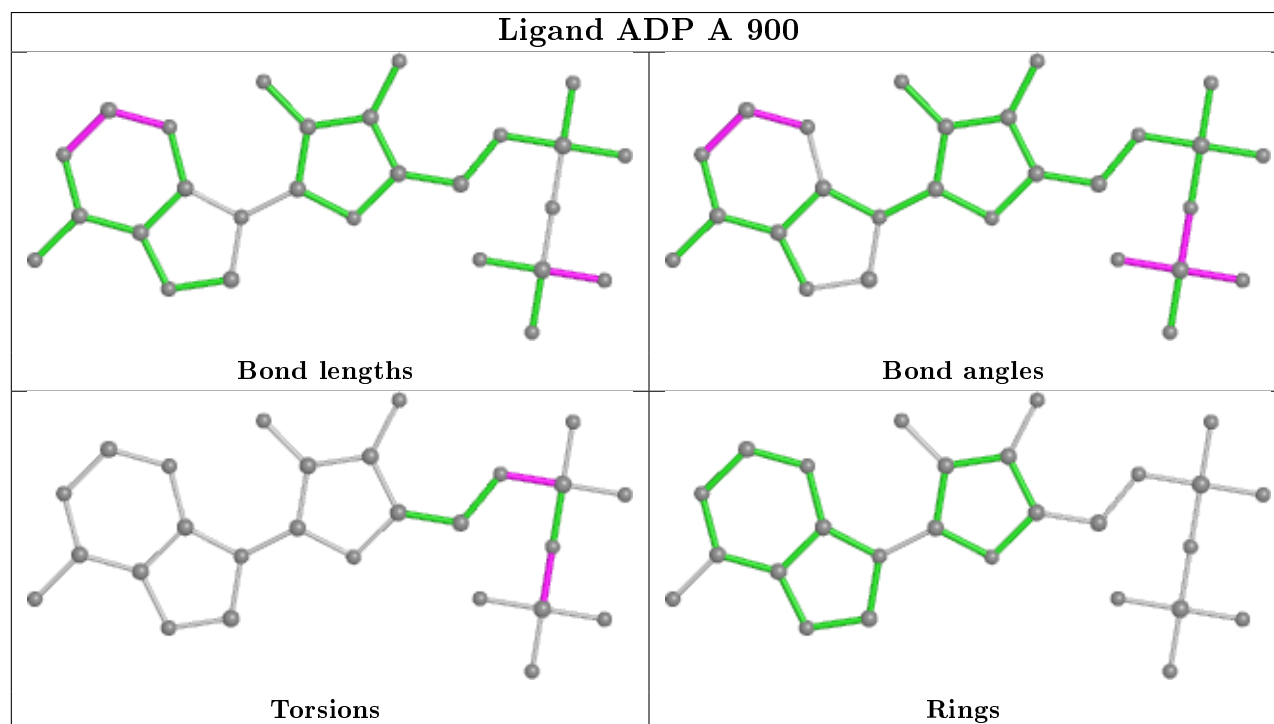
Mol	Chain	Res	Type	Atoms
3	A	900	ADP	PA-O3A-PB-O2B
3	B	901	ADP	PA-O3A-PB-O1B
3	A	900	ADP	PA-O3A-PB-O1B
3	A	900	ADP	PA-O3A-PB-O3B
3	A	900	ADP	C5'-O5'-PA-O1A
3	B	901	ADP	C5'-O5'-PA-O1A

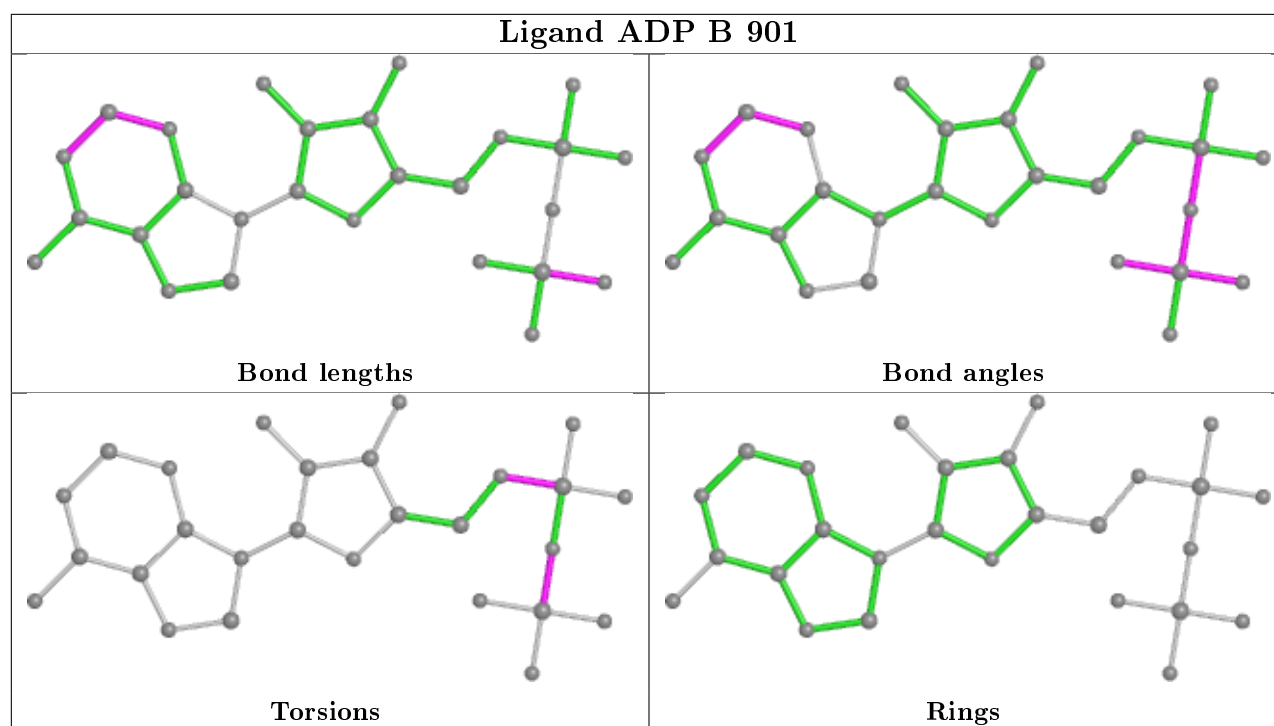
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	901	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 ⓘ

### 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.