



Full wwPDB X-ray Structure Validation Report

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
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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 types of validation reports are described at

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

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

MolProbity : 4.02b-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) : 2.36

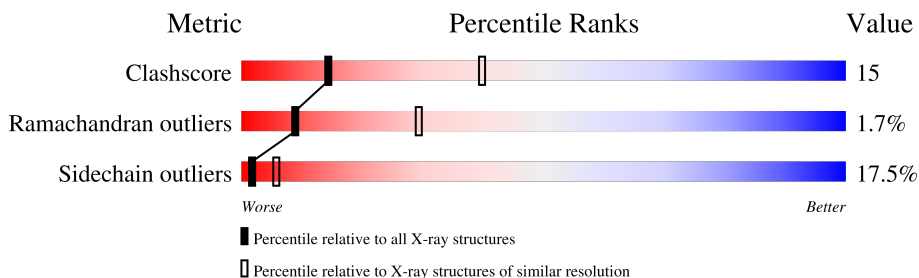
1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	922	 60% 25% 6% • 9%
1	B	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.

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

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

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 water.

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

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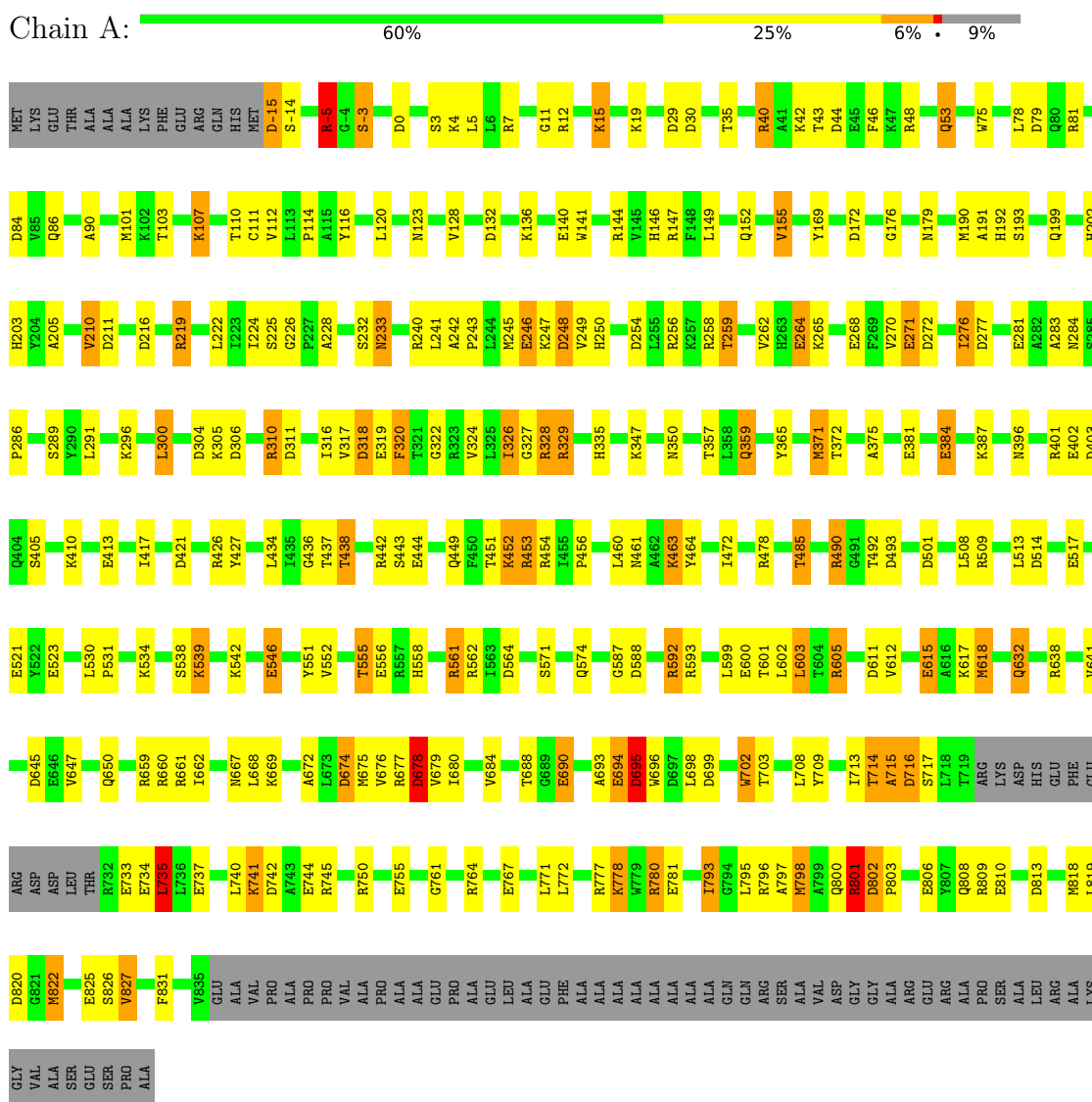
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	455	Total 455	O 455	0	0

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



- Molecule 1: PREPROTEIN TRANSLOCASE SECA 1 SUBUNIT



V835	GLU	A758	D678	E579	R490	E384	Y290	R200	M55	MET
ALA	VAL	G759	Y683	L586	D493	V391	L291	A205	P64	LYS
PRO	PRO	E760	V684	R592	D501	M397	L295	V210	L78	THR
ALA	ALA	R763	D685	R593	D505	K410	E299	D211	O79	ALA
PRO	PRO	R764	A687	L599	D506	T411	R303	S212	O80	ALA
PRO	VAL	R767	T688	E600	R507	E412	D304	D216	R81	LYS
VAL	ALA	R768	A693	T601	E510	E413	D305	M88	PHE	GLU
ALA	PRO	V770	E694	L602	E514	D421	V309	R219	ARG	GLN
ALA	ALA	L771	D695	L603	R511	D422	R310	M101	HIS	HIS
GLU	GLU	V774	V696	T604	D514	V422	D311	K107	MET	MET
PRO	PRO	L775	E697	R605	E517	V423	D318	T108	D-15	D-15
ALA	ALA	D776	L608	L608	E518	A424	E319	T108	S-14	S-14
ALA	GLU	D777	P609	P609	T518	A425	E319	C111	P-13	P-13
LEU	LEU	K778	D610	D610	F519	R426	F320	G225	D-12	D-12
ALA	ALA	V779	E520	E520	E520	K429	T321	P227	R-5	R-5
GLU	GLU	R780	E521	E521	E521	G430	G322	A228	G-4	G-4
PHE	ALA	Y784	Y522	Y522	Y522	G430	R323	D229	L2	L2
ALA	ALA	E785	K617	E523	E523	V433	V324	N118	L2	L2
ALA	ALA	Y788	M618	M618	M618	L434	L325	T129	S3	S3
ALA	ALA	E791	V619	V619	V619	L434	I326	T129	K4	K4
ALA	ALA	D716	T620	T620	T620	L436	G327	V130	L5	L5
ALA	ALA	S717	R621	R621	R621	G436	R328	Y133	L6	L6
ALA	ALA	I713	K624	K624	K624	T437	R329	R240	R7	R7
ALA	ALA	T714	E636	E636	E636	R442	R329	R240	L8	L8
ALA	ALA	A715	V637	V637	V637	S443	R329	R240	R12	R12
ALA	ALA	D718	R638	R638	R638	E444	R329	R240	K15	K15
ALA	ALA	V719	K639	K639	K639	E444	R329	R240	K18	K18
GLN	GLN	L795	Q629	Q629	Q629	S447	K347	A242	K18	K18
GLN	GLN	L796	V630	V630	V630	R448	V249	P243	A21	A21
ARG	ARG	R797	M648	M648	M648	R442	E349	P243	V24	V24
SER	SER	A797	N649	N649	N649	S443	R350	E246	K15	K15
ALA	ALA	M798	Q650	Q650	Q650	E444	Q351	K247	K15	K15
ALA	ALA	A799	R651	R651	R651	E444	T352	G143	K18	K18
VAL	VAL	R799	R652	R652	R652	E444	L353	G143	K18	K18
VAL	VAL	A800	K653	K653	K653	E444	L353	G143	K18	K18
ASP	ASP	Q800	K653	K653	K653	E444	L353	G143	K18	K18
GLY	GLY	D801	V654	V654	V654	E444	L353	G143	K18	K18
GLY	GLY	D802	L655	L655	L655	E444	L353	G143	K18	K18
ALA	ALA	P803	L655	L655	L655	E444	L353	G143	K18	K18
ARG	ARG	Y806	R659	R659	R659	E444	L353	G143	K18	K18
GLU	GLU	E807	R660	R660	R660	E444	L353	G143	K18	K18
ARG	ARG	Y807	R660	R660	R660	E444	L353	G143	K18	K18
ALA	ALA	R808	R661	R661	R661	E444	L353	G143	K18	K18
ALA	ALA	R809	R661	R661	R661	E444	L353	G143	K18	K18
PRO	PRO	E810	L662	L662	L662	E444	L353	G143	K18	K18
SER	SER	E810	L663	L663	L663	E444	L353	G143	K18	K18
ALA	ALA	M814	R669	R669	R669	E444	L353	G143	K18	K18
ALA	ALA	E734	R669	R669	R669	E444	L353	G143	K18	K18
LEU	LEU	L736	D670	D670	D670	E444	L353	G143	K18	K18
ARG	ARG	L736	Q666	Q666	Q666	E444	L353	G143	K18	K18
ALA	ALA	E737	Q666	Q666	Q666	E444	L353	G143	K18	K18
ALA	ALA	E737	Q666	Q666	Q666	E444	L353	G143	K18	K18
LYS	LYS	G821	L670	L670	L670	E444	L353	G143	K18	K18
GLY	GLY	M822	L670	L670	L670	E444	L353	G143	K18	K18
VAL	VAL	R823	Q671	Q671	Q671	E444	L353	G143	K18	K18
ALA	ALA	E824	A672	A672	A672	E444	L353	G143	K18	K18
ALA	ALA	E825	A672	A672	A672	E444	L353	G143	K18	K18
SER	SER	S826	A672	A672	A672	E444	L353	G143	K18	K18
GLU	GLU	V827	L673	L673	L673	E444	L353	G143	K18	K18
SER	SER	V827	D674	D674	D674	E444	L353	G143	K18	K18
PRO	PRO	F831	G572	G572	G572	E444	L353	G143	K18	K18
ALA	ALA	N832	R573	R573	R573	E444	L353	G143	K18	K18
			I757	I757	I757	E444	L353	G143	K18	K18

4 Data and refinement statistics

Xtrriage (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	206.20Å 206.20Å 295.41Å 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.	Xtrriage
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).

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

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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: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

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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: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

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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: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

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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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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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: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

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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: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

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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: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

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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: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

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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: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	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

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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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	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

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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

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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

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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

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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

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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

Sometimes 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

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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 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.