



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:07 PM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

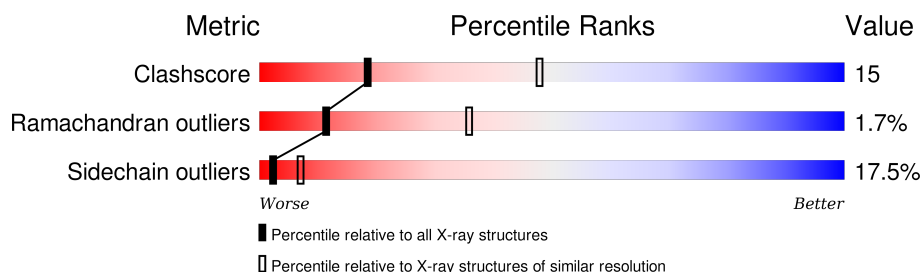
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

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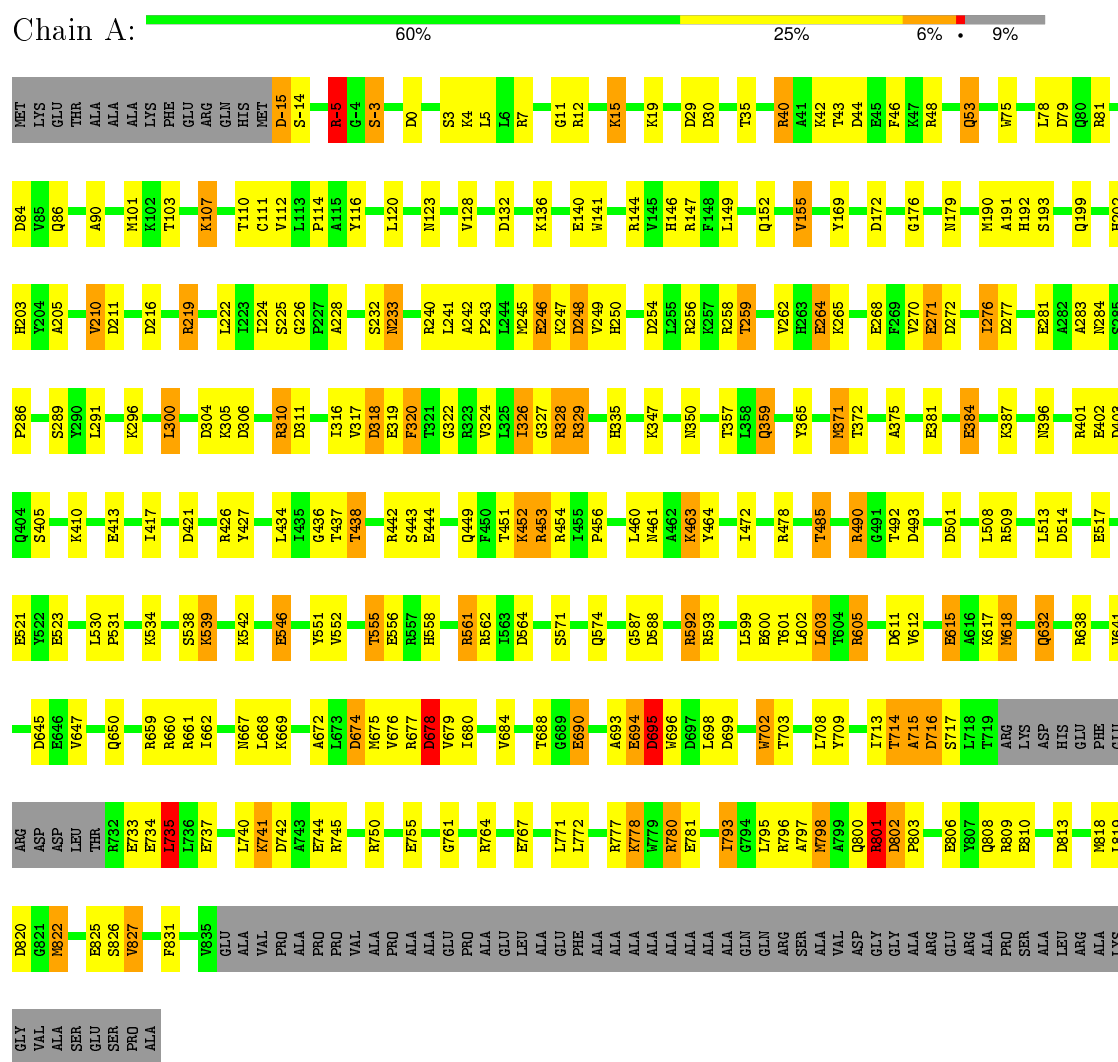
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	455	Total	O	0	0
			455	455		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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
GLU	G759	Y759	Y683	L586	D493	V391	L291	R200	P64	LYS
ALA	E760	Y684	Y684	L586	D493	V391	L295	A205	L78	THR
VAL	Y685	D685	D685	R592	D501	K397	E299	V210	Q80	ALA
PRO	Y763	R764	G686	R593	D505	K410	R303	D216	M81	ALA
ALA	Y767	Y767	A687	L599	Q506	T411	D304	S212	M83	LYS
PRO	Y768	Y768	T688	E500	R507	E412	K305	D216	M101	PHE
VAL	Y769	Y769	A693	T601	E510	E413	V309	R219	K107	GLU
ALA	Y770	Y770	D695	L602	E511	D421	R310	R219	T108	ARG
PRO	Y771	Y771	D696	L604	R514	D422	D311	L222	G111	GLN
ALA	Y774	Y774	D697	R605	D514	A423	D318	L222	V112	HIS
GLU	Y775	Y775	D698	L608	E517	A424	E319	L224	K107	MET
PRO	Y776	Y776	D699	P609	T518	A425	F320	G226	T108	D-15
ALA	Y777	Y777	A700	D610	E520	R426	T321	G227	G111	S-14
GLU	Y778	Y778	L701	D611	E521	G430	G322	A228	V116	P-13
LEU	Y779	Y779	Y702	E615	Y522	V433	G323	D229	L117	D-12
ALA	Y780	Y780	L705	A616	E523	L434	L325	S232	N118	R-5
GLU	Y784	Y784	Y709	K617	E527	G436	L326	S232	L117	G-4
PHE	Y785	Y785	Y709	K618	E528	G437	G327	N233	V130	L2
ALA	Y788	Y788	Y713	V619	E529	G438	G328	N233	Y133	R3
ALA	Y791	Y791	T714	R621	E530	G439	R329	N234	R137	K4
ALA	Y792	Y792	A715	E616	E531	G440	Q336	Y235	K136	L5
ALA	G792	Y793	D716	K624	E532	G441	Q336	A242	R137	L6
ALA	Y793	Y793	L718	V630	E533	G442	K341	P243	R137	R7
GLN	Y794	Y794	L719	E636	E534	G443	E342	E246	Y141	L8
GLN	Y795	Y795	Y719	V637	E535	G444	E343	E247	M142	R12
GLN	Y796	Y796	ARG	Y638	E536	G445	E344	D248	G143	K15
ARG	Y797	Y797	LYS	Y639	E537	G446	E345	D249	R144	K18
SER	Y798	Y798	ASP	Y640	E538	G447	E346	Y251	V145	A21
ALA	Y799	Y799	HIS	Y641	E539	G448	E347	E250	R147	Y24
VAL	Y800	Y800	GLU	Y642	E540	G449	E348	D254	L151	D30
ASP	Y801	Y801	PHE	Y643	E541	G450	E349	L255	Q152	V31
GLY	Y802	Y802	GLU	Y644	E542	G451	E350	R256	Y185	T35
ALA	Y803	Y803	ARG	Y645	E543	G452	E351	T259	D163	D36
ALA	Y804	Y804	THR	Y646	E544	G453	E352	Y260	L39	L39
ALA	Y805	Y805	ARG	Y647	E545	G454	E353	K265	R40	R40
ALA	Y806	Y806	LEU	Y648	E546	G455	E354	Y270	A41	A41
GLU	Y807	Y807	LEU	Y649	E547	G456	E355	D276	K42	K42
ARG	Y808	Y808	THR	Y650	E548	G457	E356	D277	M178	K42
ALA	Y809	Y809	ARG	Y651	E549	G458	E357	D278	M179	D44
PRO	Y810	Y810	ARG	Y652	E550	G459	E358	Y186	D184	R48
SER	Y811	Y811	LYS	Y653	E551	G460	E359	E281	L186	R49
ALA	Y812	Y812	GLY	Y654	E552	G461	E360	E282	A191	L50
ALA	Y813	Y813	GLY	Y655	E553	G462	E361	E283	D195	A51
ALA	Y814	Y814	LEU	Y656	E554	G463	E362	E284	Q53	D52
LEU	Y815	Y815	LEU	Y657	E555	G464	E363	E285	K54	K54
ARG	Y816	Y816	ARG	Y658	E556	G465	E364	E286		
ALA	Y817	Y817	LEU	Y659	E557	G466	E365	E287		
ALA	Y818	Y818	LEU	Y660	E558	G467	E366	E288		
ALA	Y819	Y819	LEU	Y661	E559	G468	E367	E289		
ALA	Y820	Y820	LEU	Y662	E560	G469	E368	E290		
LYS	Y821	Y821	LEU	Y663	E561	G470	E369	E291		
GLY	Y822	Y822	LEU	Y664	E562	G471	E370	E292		
VAL	Y823	Y823	LEU	Y665	E563	G472	E371	E293		
ALA	Y824	Y824	LEU	Y666	E564	G473	E372	E294		
ALA	Y825	Y825	LEU	Y667	E565	G474	E373	E295		
SER	Y826	Y826	LEU	Y668	E566	G475	E374	E296		
GLU	Y827	Y827	LEU	Y669	E567	G476	E375	E297		
SER	Y828	Y828	LEU	Y670	E568	G477	E376	E298		
GLU	Y829	Y829	LEU	Y671	E569	G478	E377	E299		
SER	Y830	Y830	LEU	Y672	E570	G479	E378	E300		
PRO	Y831	Y831	LEU	Y673	E571	G480	E379	E301		
ALA	Y832	Y832	LEU	Y674	E572	G481	E380	E302		
ALA	Y833	Y833	LEU	Y675	E573	G482	E381	E303		
ALA	Y834	Y834	LEU	Y676	E574	G483	E382	E304		
ALA	Y835	Y835	LEU	Y677	E575	G484	E383	E305		
ALA	Y836	Y836	LEU	Y678	E576	G485	E384	E306		
ALA	Y837	Y837	LEU	Y679	E577	G486	E385	E307		
ALA	Y838	Y838	LEU	Y680	E578	G487	E386	E308		
ALA	Y839	Y839	LEU	Y681	E579	G488	E387	E309		
ALA	Y840	Y840	LEU	Y682	E580	G489	E388	E310		
ALA	Y841	Y841	LEU	Y683	E581	G490	E389	E311		
ALA	Y842	Y842	LEU	Y684	E582	G491	E390	E312		
ALA	Y843	Y843	LEU	Y685	E583	G492	E391	E313		
ALA	Y844	Y844	LEU	Y686	E584	G493	E392	E314		
ALA	Y845	Y845	LEU	Y687	E585	G494	E393	E315		
ALA	Y846	Y846	LEU	Y688	E586	G495	E394	E316		
ALA	Y847	Y847	LEU	Y689	E587	G496	E395	E317		
ALA	Y848	Y848	LEU	Y690	E588	G497	E396	E318		
ALA	Y849	Y849	LEU	Y691	E589	G498	E397	E319		
ALA	Y850	Y850	LEU	Y692	E590	G499	E398	E320		
ALA	Y851	Y851	LEU	Y693	E591	G500	E399	E321		
ALA	Y852	Y852	LEU	Y694	E592	G501	E400	E322		
ALA	Y853	Y853	LEU	Y695	E593	G502	E401	E323		
ALA	Y854	Y854	LEU	Y696	E594	G503	E402	E324		
ALA	Y855	Y855	LEU	Y697	E595	G504	E403	E325		
ALA	Y856	Y856	LEU	Y698	E596	G505	E404	E326		
ALA	Y857	Y857	LEU	Y699	E597	G506	E405	E327		
ALA	Y858	Y858	LEU	Y700	E598	G507	E406	E328		
ALA	Y859	Y859	LEU	Y701	E599	G508	E407	E329		
ALA	Y860	Y860	LEU	Y702	E600	G509	E408	E330		
ALA	Y861	Y861	LEU	Y703	E601	G510	E409	E331		
ALA	Y862	Y862	LEU	Y704	E602	G511	E410	E332		
ALA	Y863	Y863	LEU	Y705	E603	G512	E411	E333		
ALA	Y864	Y864	LEU	Y706	E604	G513	E412	E334		
ALA	Y865	Y865	LEU	Y707	E605	G514	E413	E335		
ALA	Y866	Y866	LEU	Y708	E606	G515	E414	E336		
ALA	Y867	Y867	LEU	Y709	E607	G516	E415	E337		
ALA	Y868	Y868	LEU	Y710	E608	G517	E416	E338		
ALA	Y869	Y869	LEU	Y711	E609	G518	E417	E339		
ALA	Y870	Y870	LEU	Y712	E610	G519	E418	E340		
ALA	Y871	Y871	LEU	Y713	E611	G520	E419	E341		
ALA	Y872	Y872	LEU	Y714	E612	G521	E420	E342		
ALA	Y873	Y873	LEU	Y715	E613	G522	E421	E343		
ALA	Y874	Y874	LEU	Y716	E614	G523	E422	E344		
ALA	Y875	Y875	LEU	Y717	E615	G524	E423	E345		
ALA	Y876	Y876	LEU	Y718	E616	G525	E424	E346		
ALA	Y877	Y877	LEU	Y719	E617	G526	E425	E347		
ALA	Y878	Y878	LEU	Y720	E618	G527	E426	E348		
ALA	Y879	Y879	LEU	Y721	E619	G528	E427	E349		
ALA	Y880	Y880	LEU	Y722	E620	G529	E428	E350		
ALA	Y881	Y881	LEU	Y723	E621	G530	E429	E351		
ALA	Y882	Y882	LEU	Y724	E622	G531	E430	E352		
ALA	Y883	Y883	LEU	Y725	E623	G532	E431	E353		
ALA	Y884	Y884	LEU	Y726	E624	G533	E432	E354		
ALA	Y885	Y885	LEU	Y727	E625	G534	E433	E355		
ALA	Y886	Y886	LEU	Y728	E626	G535	E434	E356		
ALA	Y887	Y887	LEU	Y729	E627	G536	E435	E357		
ALA	Y888	Y888	LEU	Y730	E628	G537	E436	E358		
ALA	Y889	Y889	LEU	Y731	E629	G538	E437	E359		
ALA	Y890	Y890	LEU	Y732	E630	G539	E438	E360		
ALA	Y891	Y891	LEU	Y733	E631	G540	E439	E361		
ALA	Y892	Y892	LEU	Y734	E632	G541	E440	E362		
ALA	Y893	Y893	LEU	Y735	E633	G542	E441	E363		
ALA	Y894	Y894	LEU	Y736	E634	G543	E442	E364		
ALA	Y895	Y895	LEU	Y737	E635	G544	E443	E365		
ALA	Y896	Y896	LEU	Y738	E636	G545	E444	E366		
ALA	Y897	Y897	LEU	Y739	E637	G546	E445	E367		
ALA	Y898	Y898	LEU	Y740	E638	G547	E446	E368		
ALA	Y899	Y899	LEU	Y741	E639	G548	E447	E369		
ALA	Y900	Y900	LEU	Y742	E640	G549	E448	E370		
ALA	Y901	Y901	LEU	Y743	E641	G550	E449	E371		
ALA	Y902	Y902	LEU	Y744	E642	G551	E450	E372		
ALA	Y903	Y903	LEU	Y745	E643	G552	E451	E373		
ALA	Y904	Y904	LEU	Y746	E644	G553	E452	E374		
ALA	Y905	Y905	LEU	Y747	E645	G554	E453	E375		
ALA	Y906	Y906	LEU	Y748	E646	G555	E454	E376		
ALA	Y907	Y907	LEU	Y749	E647	G556	E455	E377		
ALA	Y908	Y908	LEU	Y750	E648	G557	E45			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

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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: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

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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:683:TYR:HE2	2:B:1094:HOH:O	1.64	0.79
1:B:227:PRO:HD2	2:B:1863:HOH:O	1.83	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:B:759:GLY:O	1:B:760:GLU:HB2	1.85	0.75
1:A:558:HIS:HD2	1:A:564:ASP:OD2	1.70	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:780:ARG:HD2	2:A:1503:HOH:O	1.90	0.70
1:A:144:ARG:HD2	1:A:523:GLU:OE2	1.91	0.70
1:A:461:ASN:OD1	1:A:485:THR:HG21	1.92	0.69
1:A:801:ARG:H	1:A:801:ARG:HE	1.38	0.69
1:A:611:ASP:HB3	2:A:1380:HOH:O	1.92	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:B:246:GLU:HB3	1:B:249:VAL:HB	1.75	0.68
1:A:669:LYS:HD3	1:A:764:ARG:NH2	2.08	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: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:B:559:GLU:HG2	1:B:630:VAL:CG1	2.27	0.65
1:A:326:ILE:HD13	1:B:608:LEU:HD12	1.79	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:801:ARG:HD2	1:B:802:ASP:N	2.14	0.63
1:B:490:ARG:HA	2:B:1818:HOH:O	1.99	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:326:ILE:HG13	1:A:327:GLY:N	2.15	0.61
1:A:228:ALA:HB3	2:A:1405:HOH:O	2.00	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:453:ARG:CG	1:B:453:ARG:HH11	2.14	0.59
1:B:440:VAL:O	1:B:444:GLU:HG2	2.03	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:B:248:ASP:HA	2:B:1725:HOH:O	2.02	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:116:TYR:HD1	1:B:151:LEU:HD11	1.68	0.58
1:A:112:VAL:HG13	1:A:146:HIS:CE1	2.38	0.58
1:A:219:ARG:HB3	2:A:1874:HOH:O	2.02	0.58
1:B:797:ALA:HB1	1:B:801:ARG:HD3	1.86	0.58
1:A:461:ASN:HA	1:A:485:THR:CG2	2.34	0.58
1:B:357:THR:HB	1:B:359:GLN:NE2	2.18	0.58
1:B:116:TYR:CD1	1:B:151:LEU:HD11	2.39	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:HH11	1:B:256:ARG:CB	2.18	0.56
1:B:39:LEU:HD23	1:B:148:PHE:HE1	1.70	0.56
1:B:256:ARG:HH11	1:B:256:ARG:HB2	1.71	0.56
1:B:108:THR:HG23	2:B:1651:HOH:O	2.04	0.56
1:A:410:LYS:HD2	1:A:603:LEU:HB3	1.86	0.56
1:B:649:ASN:HD22	1:B:652:ARG:HE	1.52	0.55
1:A:245:MET:CE	1:A:270:VAL:HG22	2.37	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:B:359:GLN:HE21	1:B:359:GLN:N	1.92	0.55
1:A:140:GLU:HA	1:A:147:ARG:HH22	1.71	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: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: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:B:507:ARG:HH11	1:B:507:ARG:HG3	1.71	0.54
1:A:245:MET:HE1	1:A:270:VAL:CG2	2.38	0.54
1:A:501:ASP:HB3	2:A:1786:HOH:O	2.07	0.54
1:B:425:GLU:HG2	2:B:1707:HOH:O	2.07	0.54
1:A:243:PRO:HG2	2:A:1382: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:B:4:LYS:C	1:B:6:LEU:N	2.62	0.54
1:A:755:GLU:HB3	2:A:1925:HOH:O	2.08	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:801:ARG:HB3	2:B:1437:HOH:O	2.09	0.53
1:B:694:GLU:O	1:B:696:TRP:N	2.41	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:B:227:PRO:HA	1:B:349:GLU:O	2.10	0.51
1:A:667:ASN:ND2	1:A:764:ARG:HD2	2.26	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

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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:819:LEU:HD23	1:A:822:MET:CE	2.41	0.51
1:A:675:MET:O	1:A:679:VAL:HG23	2.11	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:328:ARG:NH1	1:A:328:ARG:CG	2.61	0.50
1:A:140:GLU:HA	1:A:147:ARG:NH2	2.26	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:660:ARG:CG	2:B:1740:HOH:O	2.57	0.50
1:B:593:ARG:HD2	2:B:1701:HOH:O	2.10	0.50
1:B:677:ARG:HD3	2:B:1289:HOH:O	2.11	0.50
1:B:136:LYS:HA	1:B:155:VAL:HG11	1.93	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:B:254:ASP:HB3	1:B:259:THR:HG22	1.95	0.48
1:A:128:VAL:HA	1:A:176:GLY:O	2.13	0.48
1:A:490:ARG:HG2	2:A:1751:HOH:O	2.11	0.48
1:A:42:LYS:NZ	2:A:1285:HOH:O	2.46	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:B:421:ASP:OD1	1:B:453:ARG:NH2	2.46	0.48
1:A:688:THR:HG23	1:A:696:TRP:CZ2	2.48	0.48
1:A:357:THR:HB	1:A:359:GLN:NE2	2.29	0.48
1:A:11:GLY:HA2	2:A:1133:HOH:O	2.13	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:372:THR:CG2	1:B:375:ALA:HB2	2.43	0.47
1:B:328:ARG:HH11	1:B:796:ARG:HD2	1.79	0.47
1:B:714:THR:O	1:B:717:SER:CB	2.61	0.47
1:A:116:TYR:CZ	1:A:149:LEU:HD13	2.50	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: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: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:672:ALA:O	1:A:676:VAL:HG23	2.14	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:B:321:THR:HG22	1:B:323:ARG:HB2	1.96	0.47
1:A:713:ILE:O	1:A:714:THR:O	2.32	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: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:310:ARG:HE	1:A:310:ARG:HA	1.79	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:647:VAL:HG22	1:A:808:GLN:HG3	1.97	0.46
1:A:-5:ARG:HD3	1:A:-5:ARG:HA	1.65	0.46
1:B:716:ASP:O	1:B:717:SER:C	2.54	0.46
1:A:191:ALA:O	1:A:659:ARG:NH2	2.38	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:258:ARG:HG2	2:B:1493:HOH:O	2.15	0.45
1:B:12:ARG:NH1	2:B:1295:HOH:O	2.48	0.45
1:B:662:ILE:HG23	1:B:768:ARG:HG2	1.97	0.45
1:B:323:ARG:HD2	1:B:323:ARG:HA	1.73	0.45
1:B:163:ASP:OD1	1:B:166:ARG:NH1	2.50	0.45
1:A:587:GLY:O	1:A:592:ARG:NH1	2.48	0.45
1:A:226:GLY:O	1:A:350:ASN:HA	2.17	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:B:444:GLU:H	1:B:444:GLU:HG2	1.64	0.45
1:B:129:THR:CB	2:B:1366:HOH:O	2.64	0.45
1:A:427:TYR:CZ	1:A:456:PRO:HD2	2.51	0.45
1:A:211:ASP:OD2	1:A:562:ARG:NH1	2.46	0.45
1:B:4:LYS:HG3	2:B:1069:HOH:O	2.16	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: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:B:246:GLU:N	1:B:250:HIS:HD2	2.14	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:615:GLU:HA	2:B:1514:HOH:O	2.17	0.45
1:A:605:ARG:NH1	1:B:791:GLU:OE2	2.49	0.45
1:A:179:ASN:HB2	2:A:1827:HOH:O	2.16	0.45
1:B:532:ILE:O	1:B:535:GLU:HB2	2.15	0.45
1:A:463:LYS:HB3	1:A:464:TYR:CD1	2.52	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:617:LYS:HB2	2:A:1872:HOH:O	2.17	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:B:709:TYR:HB3	1:B:831:PHE:CD2	2.52	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:423:VAL:HG11	1:B:450:PHE:CZ	2.53	0.44
1:B:205:ALA:HB2	1:B:365:TYR:CE2	2.51	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:798:MET:HG2	2:A:1385:HOH:O	2.17	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:B:694:GLU:H	1:B:694:GLU:HG2	1.61	0.43
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:A:661:ARG:NH2	2:A:1576:HOH:O	2.51	0.43
1:A:530:LEU:HB3	1:A:531:PRO:HD3	2.00	0.43
1:B:531:PRO:HB3	2:B:1584:HOH:O	2.17	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:559:GLU:HG2	1:B:630:VAL:HG12	2.01	0.43
1:B:4:LYS:CG	2:B:1069:HOH:O	2.66	0.43
1:B:430:GLY:O	1:B:478:ARG:HB2	2.19	0.43
1:B:200:ARG:O	1:B:200:ARG:HG3	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:687:ALA:HB3	1:B:701:LEU:HD13	2.00	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:A:451:THR:C	1:A:453:ARG:H	2.22	0.43
1:A:246:GLU:N	1:A:250:HIS:HD2	2.08	0.43
1:B:328:ARG:NH1	1:B:796:ARG:HD2	2.34	0.43
1:B:678:ASP:OD1	1:B:823:LYS:HE2	2.18	0.43
1:B:463:LYS:HB3	1:B:464:TYR:CD1	2.53	0.43
1:A:90:ALA:HB1	1:A:114:PRO:HD3	2.00	0.43
1:A:798:MET:O	1:A:801:ARG:HG3	2.18	0.43
1:A:761:GLY:O	1:A:764:ARG:HB2	2.19	0.43
1:B:40:ARG:HD3	2:B:1825:HOH:O	2.18	0.43
1:A:233:ASN:ND2	1:A:233:ASN:N	2.66	0.43
1:A:438:THR:HB	1:A:556:GLU:CG	2.49	0.42
1:B:6:LEU:C	1:B:8:LEU:N	2.73	0.42
1:A:329:ARG:HB3	1:A:335:HIS:ND1	2.34	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: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:223:ILE:HG12	1:B:355:THR:CG2	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:797:ALA:HA	1:A:801:ARG:HD3	2.01	0.42
1:A:169:TYR:CE1	1:A:199:GLN:HG2	2.55	0.42
1:A:103:THR:HA	2:A:1132:HOH:O	2.18	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: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:190:MET:HE1	1:A:224:ILE:HD13	2.01	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:HA	1:B:-5:ARG:HD3	1.65	0.42
1:B:222:LEU:O	1:B:355:THR:HG22	2.20	0.41
1:A:561:ARG:O	1:A:561:ARG:HG3	2.19	0.41
1:B:223:ILE:HG23	1:B:352:THR:HG23	2.02	0.41
1:A:660:ARG:NH1	2:A:1929:HOH:O	2.51	0.41
1:A:451:THR:C	1:A:453:ARG:N	2.74	0.41
1:B:453:ARG:HG3	1:B:453:ARG:HH11	1.84	0.41
1:B:133:TYR:CZ	1:B:137:ARG:HD3	2.55	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:B:802:ASP:HA	1:B:803:PRO:HD2	1.95	0.41
1:B:116:TYR:HD1	1:B:151:LEU:CD1	2.31	0.41
1:A:202:HIS:O	1:A:365:TYR:HA	2.21	0.41
1:B:424:ALA:HB2	1:B:455:ILE:HD11	2.01	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:381:GLU:OE2	1:B:638:ARG:HD2	2.20	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:381:GLU:OE2	1:A:638:ARG:HD2	2.21	0.41
1:B:552:VAL:HG23	1:B:571:SER:HB2	2.03	0.41
1:B:152:GLN:HG2	2:B:1365:HOH:O	2.21	0.41
1:A:268:GLU:HA	1:A:271:GLU: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:653:LYS:HE3	2:B:1235:HOH:O	2.21	0.40
1:B:326:ILE:HG13	1:B:795:LEU:HD13	2.04	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:514:ASP:HB3	1:B:517:GLU:HB2	2.03	0.40
1:B:397:MET:HE2	2:B:1413:HOH:O	2.21	0.40
1:B:551:TYR:HD1	1:B:579:GLU:HB3	1.86	0.40
1:A:283:ALA:O	1:A:284:ASN:CB	2.68	0.40
1:B:785:GLU:HG3	2:B:1130:HOH:O	2.20	0.40
1:A:702:TRP:CD1	1:A:714:THR:HG23	2.57	0.40
1:A:603:LEU:HA	1:A:603:LEU:HD12	1.96	0.40
1:A:101:MET:CE	1:A:371:MET:CE	2.99	0.40
1:B:672:ALA:HB2	1:B:767:GLU:HG2	2.03	0.40
1:A:317:VAL:HG12	1:A:324:VAL:HA	2.04	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%)	12	38
1	B	834/922 (90%)	758 (91%)	60 (7%)	16 (2%)	10	32
All	All	1669/1844 (90%)	1523 (91%)	117 (7%)	29 (2%)	11	36

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 ⓘ

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	7
1	B	697/755 (92%)	572 (82%)	125 (18%)	2	6
All	All	1393/1510 (92%)	1149 (82%)	244 (18%)	2	7

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

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

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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 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.