



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:04 PM UTC

PDB ID : 3U95 / pdb_00003u95
Title : Crystal structure of a putative alpha-glucosidase from *Thermotoga neapolitana*
Authors : Ha, N.C.; Jun, S.Y.; Yun, B.Y.; Yoon, B.Y.; Piao, S.
Deposited on : 2011-10-17
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

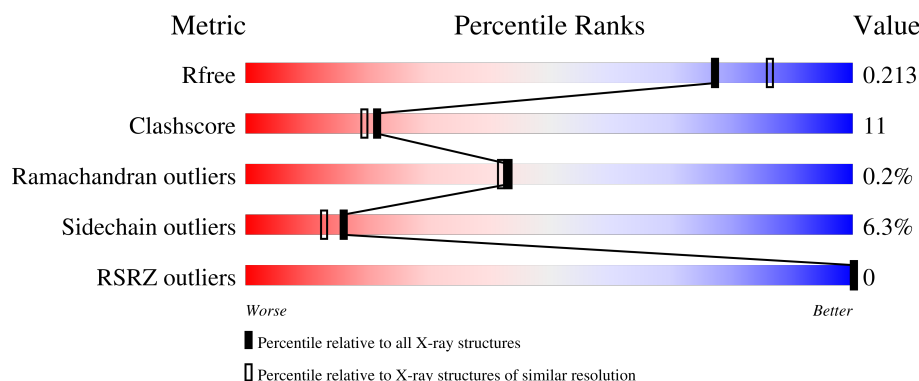
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	477	
1	B	477	
1	C	477	
1	D	477	
1	E	477	

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Mol	Chain	Length	Quality of chain
1	F	477	76% 19% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25816 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 Glycoside hydrolase, family 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3894	2494	679	709	12			
1	B	469	Total	C	N	O	S	0	0	0
			3902	2498	681	711	12			
1	C	464	Total	C	N	O	S	0	0	0
			3860	2473	673	703	11			
1	D	468	Total	C	N	O	S	0	0	0
			3894	2494	679	709	12			
1	E	466	Total	C	N	O	S	0	0	0
			3877	2483	675	707	12			
1	F	469	Total	C	N	O	S	0	0	0
			3902	2498	681	711	12			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	THR	MET	conflict	UNP B9KAM3
A	470	LEU	-	expression tag	UNP B9KAM3
A	471	GLU	-	expression tag	UNP B9KAM3
A	472	HIS	-	expression tag	UNP B9KAM3
A	473	HIS	-	expression tag	UNP B9KAM3
A	474	HIS	-	expression tag	UNP B9KAM3
A	475	HIS	-	expression tag	UNP B9KAM3
A	476	HIS	-	expression tag	UNP B9KAM3
A	477	HIS	-	expression tag	UNP B9KAM3
B	416	THR	MET	conflict	UNP B9KAM3
B	470	LEU	-	expression tag	UNP B9KAM3
B	471	GLU	-	expression tag	UNP B9KAM3
B	472	HIS	-	expression tag	UNP B9KAM3
B	473	HIS	-	expression tag	UNP B9KAM3
B	474	HIS	-	expression tag	UNP B9KAM3
B	475	HIS	-	expression tag	UNP B9KAM3
B	476	HIS	-	expression tag	UNP B9KAM3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	HIS	-	expression tag	UNP B9KAM3
C	416	THR	MET	conflict	UNP B9KAM3
C	470	LEU	-	expression tag	UNP B9KAM3
C	471	GLU	-	expression tag	UNP B9KAM3
C	472	HIS	-	expression tag	UNP B9KAM3
C	473	HIS	-	expression tag	UNP B9KAM3
C	474	HIS	-	expression tag	UNP B9KAM3
C	475	HIS	-	expression tag	UNP B9KAM3
C	476	HIS	-	expression tag	UNP B9KAM3
C	477	HIS	-	expression tag	UNP B9KAM3
D	416	THR	MET	conflict	UNP B9KAM3
D	470	LEU	-	expression tag	UNP B9KAM3
D	471	GLU	-	expression tag	UNP B9KAM3
D	472	HIS	-	expression tag	UNP B9KAM3
D	473	HIS	-	expression tag	UNP B9KAM3
D	474	HIS	-	expression tag	UNP B9KAM3
D	475	HIS	-	expression tag	UNP B9KAM3
D	476	HIS	-	expression tag	UNP B9KAM3
D	477	HIS	-	expression tag	UNP B9KAM3
E	416	THR	MET	conflict	UNP B9KAM3
E	470	LEU	-	expression tag	UNP B9KAM3
E	471	GLU	-	expression tag	UNP B9KAM3
E	472	HIS	-	expression tag	UNP B9KAM3
E	473	HIS	-	expression tag	UNP B9KAM3
E	474	HIS	-	expression tag	UNP B9KAM3
E	475	HIS	-	expression tag	UNP B9KAM3
E	476	HIS	-	expression tag	UNP B9KAM3
E	477	HIS	-	expression tag	UNP B9KAM3
F	416	THR	MET	conflict	UNP B9KAM3
F	470	LEU	-	expression tag	UNP B9KAM3
F	471	GLU	-	expression tag	UNP B9KAM3
F	472	HIS	-	expression tag	UNP B9KAM3
F	473	HIS	-	expression tag	UNP B9KAM3
F	474	HIS	-	expression tag	UNP B9KAM3
F	475	HIS	-	expression tag	UNP B9KAM3
F	476	HIS	-	expression tag	UNP B9KAM3
F	477	HIS	-	expression tag	UNP B9KAM3

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

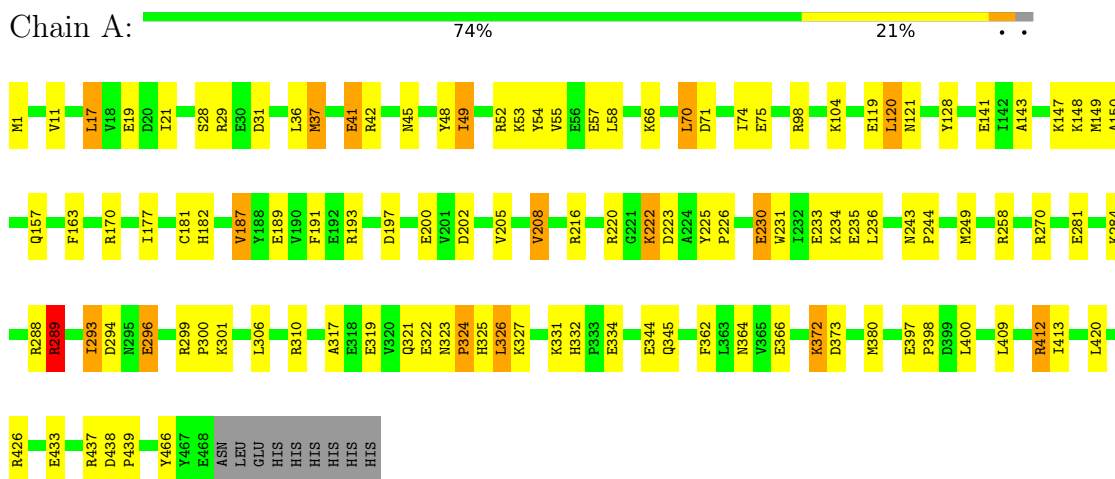
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	444	Total 444	O 444	0	0
3	B	402	Total 402	O 402	0	0
3	C	393	Total 393	O 393	0	0
3	D	450	Total 450	O 450	0	0
3	E	431	Total 431	O 431	0	0
3	F	361	Total 361	O 361	0	0

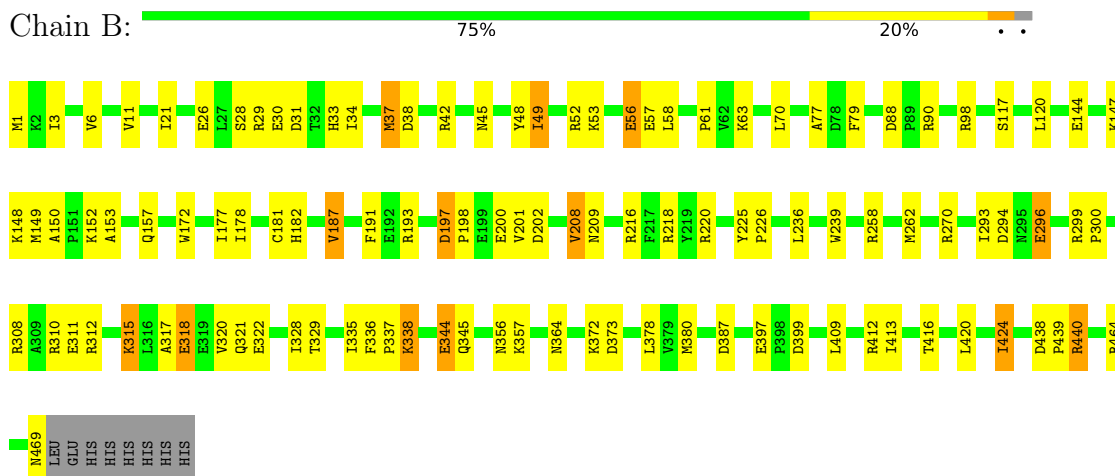
3 Residue-property plots

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 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.

- Molecule 1: Glycoside hydrolase, family 4



- Molecule 1: Glycoside hydrolase, family 4



- Molecule 1: Glycoside hydrolase, family 4



M469	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	M1
LEU	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	M149																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
GLU	P323	P324	P325	P326	P327	P328	P329	P330	P331	P332	P333	P334	P335	P336	P337	P338	P339	P340	P341	P342	P343	P344	P345	P346	P347	P348	P349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359	P360	P361	P362	P363	P364	P365	P366	P367	P368	P369	P370	P371	P372	P373	P374	P375	P376	P377	P378	P379	P380	P381	P382	P383	P384	P385	P386	P387	P388	P389	P390	P391	P392	P393	P394	P395	P396	P397	P398	P399	P400	P401	P402	P403	P404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420	P421	P422	P423	P424	P425	P426	P427	P428	P429	P430	P431	P432	P433	P434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470	P471	P472	P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	M149																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
HIS	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	M149																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
HIS	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	M149																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
HIS	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	154.53Å 154.53Å 139.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.90 – 2.00 40.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.90-2.00) 98.9 (40.90-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.185 , 0.222 0.180 , 0.213	Depositor DCC
R_{free} test set	1985 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.024 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25816	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0314e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/3994	0.78	5/5407 (0.1%)
1	B	0.45	0/4002	0.78	7/5418 (0.1%)
1	C	0.45	0/3957	0.75	2/5355 (0.0%)
1	D	0.47	0/3994	0.78	4/5407 (0.1%)
1	E	0.47	0/3974	0.76	1/5377 (0.0%)
1	F	0.44	0/4002	0.75	2/5418 (0.0%)
All	All	0.46	0/23923	0.77	21/32382 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	ASP	CA-C-N	6.30	126.50	119.32
1	B	438	ASP	C-N-CA	6.30	126.50	119.32
1	B	150	ALA	CA-C-N	5.99	125.69	119.82
1	B	150	ALA	C-N-CA	5.99	125.69	119.82
1	D	11	VAL	N-CA-C	5.78	115.97	110.42
1	A	11	VAL	N-CA-C	5.64	115.77	110.30
1	F	150	ALA	CA-C-N	5.55	125.26	119.82
1	F	150	ALA	C-N-CA	5.55	125.26	119.82
1	B	11	VAL	N-CA-C	5.52	115.97	110.23
1	C	438	ASP	CA-C-N	5.44	125.78	119.47
1	C	438	ASP	C-N-CA	5.44	125.78	119.47
1	B	197	ASP	CA-C-N	5.32	125.64	119.47
1	B	197	ASP	C-N-CA	5.32	125.64	119.47
1	D	324	PRO	N-CA-C	-5.30	103.75	111.33
1	A	332	HIS	CA-C-N	5.26	124.58	118.85
1	A	332	HIS	C-N-CA	5.26	124.58	118.85
1	D	150	ALA	CA-C-N	5.21	124.93	119.82
1	D	150	ALA	C-N-CA	5.21	124.93	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ALA	CA-C-N	5.18	124.90	119.82
1	A	150	ALA	C-N-CA	5.18	124.90	119.82
1	E	11	VAL	N-CA-C	5.18	115.32	110.30

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	3894	0	3847	91	0
1	B	3902	0	3853	80	0
1	C	3860	0	3814	98	0
1	D	3894	0	3848	75	0
1	E	3877	0	3832	77	0
1	F	3902	0	3853	86	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	444	0	0	16	0
3	B	402	0	0	12	0
3	C	393	0	0	19	0
3	D	450	0	0	14	0
3	E	431	0	0	13	0
3	F	361	0	0	21	0
All	All	25816	0	23047	500	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 (500) 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:289:ARG:HH21	1:A:289:ARG:HG3	1.15	1.09
1:C:429:LYS:HG3	3:D:2410:HOH:O	1.48	1.09
1:A:182:HIS:CE1	1:A:344:GLU:HG3	1.94	1.03
1:F:289:ARG:HG2	3:F:2213:HOH:O	1.58	1.03
1:A:182:HIS:HE1	1:A:344:GLU:HG3	1.25	1.02
1:D:258:ARG:HH11	1:D:258:ARG:HG2	1.21	1.00
1:A:222:LYS:HD3	1:A:223:ASP:H	1.23	1.00
1:F:49:ILE:HD11	1:F:317:ALA:HB1	1.43	0.98
1:A:182:HIS:CE1	1:A:345:GLN:H	1.79	0.98
1:E:461:GLU:OE2	3:E:2103:HOH:O	1.82	0.96
1:F:48:TYR:OH	3:F:1780:HOH:O	1.85	0.95
1:D:308:ARG:NH2	3:D:2063:HOH:O	1.99	0.93
1:A:310:ARG:NH1	3:A:2217:HOH:O	1.96	0.92
1:D:429:LYS:HG3	3:D:1953:HOH:O	1.68	0.92
1:B:201:VAL:N	3:B:2090:HOH:O	1.89	0.92
1:F:26:GLU:OE1	3:F:829:HOH:O	1.91	0.89
1:A:230:GLU:OE2	1:A:234:LYS:NZ	2.06	0.88
1:D:219:TYR:OH	3:D:1779:HOH:O	1.91	0.88
1:C:270:ARG:HD2	1:C:294:ASP:OD2	1.75	0.87
1:A:49:ILE:HD11	1:A:317:ALA:HB1	1.57	0.87
1:E:245:TRP:CE2	1:E:293:ILE:HD12	2.12	0.84
1:D:285:LYS:NZ	3:D:2277:HOH:O	2.10	0.84
1:A:310:ARG:NH2	3:A:2217:HOH:O	2.08	0.83
1:B:182:HIS:CE1	1:B:344:GLU:HA	2.14	0.82
1:C:37:MET:HE2	1:C:38:ASP:N	1.94	0.81
1:B:182:HIS:CE1	1:B:345:GLN:HG3	2.16	0.80
1:B:310:ARG:NH1	1:B:311:GLU:OE1	2.13	0.80
1:B:338:LYS:H	1:B:338:LYS:HZ2	1.27	0.80
1:A:412:ARG:HD3	3:A:1649:HOH:O	1.81	0.80
1:A:222:LYS:HD3	1:A:223:ASP:N	1.96	0.80
1:C:193:ARG:HD2	3:C:1683:HOH:O	1.80	0.80
1:B:29:ARG:NH2	1:B:31:ASP:OD1	2.15	0.80
1:B:338:LYS:H	1:B:338:LYS:NZ	1.81	0.79
1:F:42:ARG:NE	3:F:1478:HOH:O	2.14	0.79
1:A:197:ASP:HB3	1:A:200:GLU:HG3	1.62	0.79
1:B:469:ASN:O	3:B:2453:HOH:O	2.01	0.79
1:E:270:ARG:HD2	1:E:294:ASP:OD2	1.84	0.78
1:A:289:ARG:HH21	1:A:289:ARG:CG	1.96	0.78
1:A:289:ARG:HG3	1:A:289:ARG:NH2	1.96	0.78
3:E:1090:HOH:O	1:F:429:LYS:HG3	1.82	0.78
1:F:182:HIS:HE2	1:F:345:GLN:H	1.32	0.78
1:A:200:GLU:OE2	1:A:220:ARG:NH2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:NH1	3:D:1576:HOH:O	2.17	0.76
1:E:200:GLU:OE2	3:E:1923:HOH:O	2.03	0.75
1:E:52:ARG:NH2	3:E:2168:HOH:O	2.19	0.75
1:B:198:PRO:C	3:B:2090:HOH:O	2.30	0.74
1:C:75:GLU:HB2	1:C:149:MET:HE2	1.69	0.74
1:C:468:GLU:OE2	3:C:2345:HOH:O	2.06	0.74
1:D:258:ARG:HG2	1:D:258:ARG:NH1	1.96	0.74
1:A:270:ARG:HD2	1:A:294:ASP:OD2	1.86	0.74
1:E:111:TYR:HE1	1:E:450:VAL:HG21	1.52	0.74
1:A:48:TYR:CZ	1:A:52:ARG:HD2	2.23	0.74
1:A:296:GLU:HG2	3:A:1091:HOH:O	1.88	0.74
1:D:33:HIS:CE1	1:D:63:LYS:HD2	2.23	0.73
1:E:446:GLN:O	1:E:450:VAL:HG23	1.87	0.73
1:E:111:TYR:CE1	1:E:450:VAL:HG21	2.23	0.73
1:F:310:ARG:NH1	1:F:311:GLU:OE1	2.21	0.73
1:F:464:ARG:NH2	3:F:499:HOH:O	2.18	0.73
1:A:409:LEU:O	1:A:413:ILE:HD13	1.88	0.72
1:D:270:ARG:HD2	1:D:294:ASP:OD2	1.90	0.72
1:D:37:MET:HE3	1:D:70:LEU:HA	1.70	0.72
1:C:296:GLU:HG2	3:C:1078:HOH:O	1.87	0.72
1:D:193:ARG:NH2	3:D:1383:HOH:O	2.05	0.72
1:F:71:ASP:CG	3:F:2121:HOH:O	2.32	0.71
1:B:270:ARG:HD2	1:B:294:ASP:OD2	1.90	0.71
1:D:42:ARG:HG2	1:D:42:ARG:HH21	1.55	0.70
1:A:310:ARG:CZ	3:A:2217:HOH:O	2.30	0.70
1:E:77:ALA:O	1:E:153:ALA:HB2	1.92	0.70
1:E:281:GLU:OE1	3:E:549:HOH:O	2.10	0.70
1:A:202:ASP:OD2	3:A:2110:HOH:O	2.10	0.69
1:C:57:GLU:OE1	1:C:329:THR:OG1	2.09	0.69
1:D:322:GLU:O	1:D:323:ASN:HB2	1.93	0.69
1:D:312:ARG:NH2	3:D:568:HOH:O	2.25	0.68
1:E:310:ARG:HD3	3:E:2306:HOH:O	1.92	0.68
1:B:197:ASP:O	3:B:2090:HOH:O	2.11	0.68
1:D:258:ARG:HH11	1:D:258:ARG:CG	2.03	0.68
1:A:181:CYS:C	1:A:182:HIS:CD2	2.72	0.68
1:B:33:HIS:NE2	1:B:63:LYS:HD2	2.08	0.68
1:E:327:LYS:HD2	1:E:330:GLU:OE2	1.94	0.68
1:B:45:ASN:O	1:B:49:ILE:HG22	1.94	0.68
1:A:49:ILE:CD1	1:A:317:ALA:HB1	2.25	0.67
1:E:124:SER:O	1:E:125:THR:HG22	1.94	0.67
1:F:327:LYS:HB3	1:F:330:GLU:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:LYS:NZ	1:E:75:GLU:O	2.22	0.67
1:F:53:LYS:NZ	1:F:57:GLU:OE2	2.27	0.67
1:E:1:MET:HE1	1:E:79:PHE:HE2	1.60	0.66
1:E:109:HIS:HB3	1:E:450:VAL:HG22	1.77	0.66
1:B:58:LEU:O	3:B:2161:HOH:O	2.14	0.66
1:C:187:VAL:HG13	1:C:191:PHE:CZ	2.30	0.66
1:E:426:ARG:HG2	1:E:466:TYR:CZ	2.30	0.66
1:A:326:LEU:HD21	1:A:331:LYS:HD2	1.78	0.66
1:D:41:GLU:HG3	1:D:42:ARG:N	2.10	0.66
1:D:255:ASP:OD1	1:D:258:ARG:NH2	2.28	0.66
1:D:446:GLN:O	1:D:450:VAL:HG23	1.96	0.66
1:F:117:SER:O	1:F:440:ARG:NH2	2.29	0.65
1:F:150:ALA:N	1:F:151:PRO:HD3	2.11	0.65
1:D:86:PRO:O	1:D:98:ARG:NH1	2.28	0.65
1:E:1:MET:N	1:E:31:ASP:O	2.29	0.65
1:E:120:LEU:HB3	1:E:412:ARG:HD3	1.77	0.65
1:F:57:GLU:OE1	1:F:329:THR:OG1	2.11	0.65
1:F:254:MET:O	1:F:258:ARG:HG2	1.96	0.65
1:B:49:ILE:HD11	1:B:320:VAL:HB	1.79	0.65
1:B:409:LEU:O	1:B:413:ILE:HG12	1.97	0.65
1:C:53:LYS:NZ	1:C:57:GLU:OE2	2.30	0.65
1:C:141:GLU:OE2	3:C:2095:HOH:O	2.13	0.65
1:B:372:LYS:HD2	1:B:373:ASP:OD2	1.97	0.65
1:F:145:LYS:NZ	3:F:2121:HOH:O	2.30	0.65
1:C:182:HIS:NE2	1:C:345:GLN:N	2.45	0.64
1:A:181:CYS:C	1:A:182:HIS:HD2	2.06	0.64
1:F:33:HIS:NE2	1:F:63:LYS:HD2	2.12	0.64
1:A:181:CYS:O	1:A:182:HIS:HD2	1.80	0.64
1:A:284:LYS:O	1:A:288:ARG:HA	1.97	0.63
1:A:281:GLU:OE2	3:C:570:HOH:O	2.16	0.63
1:D:324:PRO:O	1:D:325:HIS:HB3	1.99	0.63
1:B:193:ARG:HH12	1:B:239:TRP:CD1	2.18	0.62
1:B:200:GLU:N	3:B:2090:HOH:O	2.33	0.62
1:D:208:VAL:HG11	1:D:412:ARG:HG2	1.80	0.62
1:C:98:ARG:NH1	3:C:558:HOH:O	2.33	0.62
1:E:53:LYS:HD2	1:E:57:GLU:OE2	1.99	0.62
1:B:312:ARG:O	1:B:315:LYS:HE2	2.00	0.62
1:F:233:GLU:HG2	1:F:234:LYS:HD3	1.81	0.62
1:C:29:ARG:HA	1:C:61:PRO:HG2	1.81	0.62
1:D:200:GLU:OE1	1:D:220:ARG:NH1	2.32	0.62
1:D:152:LYS:HB3	3:D:2427:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ILE:N	1:B:328:ILE:HD12	2.15	0.61
1:D:37:MET:HE3	1:D:70:LEU:CA	2.29	0.61
1:B:328:ILE:HD12	1:B:328:ILE:H	1.66	0.61
1:E:296:GLU:HG2	3:E:507:HOH:O	1.99	0.61
1:B:182:HIS:NE2	1:B:344:GLU:HG3	2.15	0.61
1:D:340:ARG:NH1	1:D:341:LEU:O	2.34	0.61
1:B:182:HIS:CE1	1:B:345:GLN:N	2.69	0.60
1:A:193:ARG:NH2	3:A:747:HOH:O	2.33	0.60
1:B:320:VAL:HG22	1:B:328:ILE:HD11	1.83	0.60
1:B:152:LYS:NZ	3:B:2019:HOH:O	2.33	0.60
1:E:85:TYR:OH	1:E:125:THR:OG1	2.18	0.60
1:E:442:LYS:NZ	1:F:442:LYS:HE2	2.15	0.60
1:F:372:LYS:O	1:F:373:ASP:HB2	2.01	0.60
1:A:53:LYS:HE3	1:A:57:GLU:OE2	2.02	0.60
1:A:98:ARG:HD2	1:A:128:TYR:OH	2.02	0.60
1:C:308:ARG:HG2	1:C:308:ARG:HH11	1.67	0.59
1:B:378:LEU:HD21	1:B:413:ILE:HD12	1.84	0.59
1:D:111:TYR:CE1	1:D:450:VAL:HG21	2.36	0.59
1:E:45:ASN:OD1	1:E:66:LYS:NZ	2.36	0.59
1:A:141:GLU:OE1	3:A:625:HOH:O	2.17	0.59
1:F:42:ARG:CZ	3:F:1478:HOH:O	2.49	0.59
1:F:145:LYS:HD3	3:F:2121:HOH:O	2.01	0.59
1:D:324:PRO:O	1:D:325:HIS:CB	2.51	0.59
1:E:49:ILE:HD11	1:E:317:ALA:O	2.02	0.59
1:F:75:GLU:HG2	3:F:2235:HOH:O	2.03	0.59
1:B:98:ARG:NH2	3:B:1651:HOH:O	1.88	0.59
1:B:328:ILE:HG22	1:B:336:PHE:CD2	2.38	0.59
1:E:109:HIS:CB	1:E:450:VAL:HG22	2.32	0.59
1:F:187:VAL:HG22	1:F:191:PHE:CZ	2.38	0.58
1:F:202:ASP:HB3	1:F:218:ARG:HB2	1.84	0.58
1:B:372:LYS:O	1:B:373:ASP:HB2	2.04	0.58
1:B:148:LYS:HE3	1:B:149:MET:HE2	1.86	0.58
1:C:219:TYR:CE2	1:C:220:ARG:HG3	2.39	0.58
1:F:426:ARG:HG2	1:F:466:TYR:CZ	2.39	0.57
1:F:397:GLU:HA	1:F:398:PRO:C	2.28	0.57
1:B:293:ILE:HG22	3:B:1664:HOH:O	2.03	0.57
1:C:40:HIS:CE1	1:C:43:ARG:HG3	2.38	0.57
1:C:37:MET:HE2	1:C:38:ASP:CA	2.35	0.57
1:C:114:GLY:HA3	3:C:635:HOH:O	2.04	0.57
1:D:20:ASP:HB2	1:D:347:ILE:HG13	1.85	0.57
1:D:372:LYS:O	1:D:373:ASP:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:OE2	1:A:331:LYS:NZ	2.38	0.57
1:E:442:LYS:HZ2	1:F:442:LYS:HE2	1.67	0.57
1:B:1:MET:HE2	1:B:3:ILE:CG1	2.35	0.57
1:F:322:GLU:O	1:F:324:PRO:HD3	2.04	0.57
1:D:17:LEU:O	1:D:21:ILE:HG13	2.05	0.56
1:C:49:ILE:HD11	1:C:317:ALA:HB1	1.87	0.56
1:D:426:ARG:HG2	1:D:466:TYR:CZ	2.40	0.56
1:C:48:TYR:CZ	1:C:52:ARG:HD2	2.41	0.56
1:C:48:TYR:OH	1:C:52:ARG:NH1	2.34	0.56
1:D:409:LEU:O	1:D:413:ILE:HG23	2.06	0.56
1:C:187:VAL:HG13	1:C:191:PHE:CE2	2.41	0.56
1:F:270:ARG:HD2	1:F:294:ASP:OD2	2.05	0.56
1:B:30:GLU:HA	1:B:61:PRO:O	2.04	0.55
1:C:426:ARG:HG2	1:C:466:TYR:CZ	2.41	0.55
1:A:243:ASN:HB2	1:A:244:PRO:CD	2.36	0.55
1:E:48:TYR:CG	1:E:66:LYS:HD3	2.41	0.55
1:C:193:ARG:HG3	1:C:249:MET:HG3	1.89	0.55
1:F:220:ARG:HD3	3:F:2280:HOH:O	2.07	0.55
1:A:200:GLU:HB3	1:A:220:ARG:HH12	1.71	0.55
1:A:299:ARG:HB3	1:A:300:PRO:HD3	1.88	0.55
1:C:223:ASP:O	1:C:226:PRO:HD2	2.05	0.55
1:E:397:GLU:HA	1:E:398:PRO:C	2.32	0.55
1:D:172:TRP:CE2	1:D:424:ILE:HD12	2.41	0.55
1:E:400:LEU:HD13	1:E:409:LEU:HD11	1.88	0.55
1:A:397:GLU:HA	1:A:398:PRO:C	2.31	0.55
1:A:426:ARG:HG2	1:A:466:TYR:CZ	2.41	0.55
1:D:360:ARG:HD3	3:D:1473:HOH:O	2.07	0.55
1:A:334:GLU:HB2	3:A:2157:HOH:O	2.06	0.55
1:C:119:GLU:O	1:C:120:LEU:HB2	2.06	0.55
1:C:58:LEU:HD21	1:C:338:LYS:HG2	1.89	0.55
1:C:372:LYS:O	1:C:373:ASP:HB2	2.07	0.55
1:F:181:CYS:C	1:F:182:HIS:ND1	2.65	0.54
1:A:119:GLU:O	1:A:120:LEU:HB2	2.07	0.54
1:F:378:LEU:HD21	1:F:413:ILE:CD1	2.38	0.54
1:A:230:GLU:CD	1:A:234:LYS:HZ1	2.15	0.54
1:A:372:LYS:O	1:A:373:ASP:HB2	2.07	0.54
1:E:33:HIS:CD2	3:E:1967:HOH:O	2.61	0.54
1:F:41:GLU:HG3	1:F:42:ARG:N	2.22	0.54
1:F:119:GLU:O	1:F:120:LEU:HB2	2.08	0.54
1:E:1:MET:HE1	1:E:79:PHE:CE2	2.42	0.54
1:E:321:GLN:HB3	1:E:322:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLU:HB3	1:C:234:LYS:HD2	1.90	0.53
1:F:335:ILE:C	1:F:337:PRO:HD3	2.33	0.53
1:A:41:GLU:HG3	1:A:42:ARG:N	2.22	0.53
1:C:312:ARG:NH1	3:C:2122:HOH:O	2.41	0.53
1:B:42:ARG:HA	1:B:42:ARG:NE	2.24	0.53
1:B:182:HIS:CE1	1:B:345:GLN:H	2.26	0.53
1:D:45:ASN:O	1:D:49:ILE:HG12	2.08	0.53
1:F:182:HIS:NE2	1:F:344:GLU:HG3	2.24	0.53
1:E:129:VAL:O	1:E:130:LEU:HB2	2.09	0.53
1:C:234:LYS:HD2	1:C:234:LYS:N	2.24	0.53
1:B:193:ARG:NH2	3:B:1855:HOH:O	2.42	0.53
1:D:243:ASN:HB2	1:D:244:PRO:HD2	1.90	0.53
1:B:26:GLU:OE1	1:B:26:GLU:N	2.42	0.53
1:B:193:ARG:HH12	1:B:239:TRP:NE1	2.06	0.52
1:B:216:ARG:HD3	1:B:397:GLU:O	2.09	0.52
1:C:98:ARG:NE	3:C:1375:HOH:O	2.43	0.52
1:A:182:HIS:CD2	1:A:345:GLN:HE21	2.26	0.52
1:A:71:ASP:O	1:A:149:MET:HE1	2.09	0.52
1:E:245:TRP:NE1	1:E:293:ILE:HD12	2.23	0.52
1:A:98:ARG:NH2	3:A:1053:HOH:O	2.42	0.52
1:C:222:LYS:HG2	1:C:223:ASP:H	1.74	0.52
1:E:80:ILE:HD12	1:E:146:MET:SD	2.50	0.52
1:F:372:LYS:HA	3:F:2232:HOH:O	2.10	0.52
1:A:1:MET:N	1:A:31:ASP:O	2.42	0.52
1:C:49:ILE:HD11	1:C:317:ALA:C	2.34	0.52
1:D:33:HIS:HE1	1:D:63:LYS:HD2	1.71	0.52
1:D:42:ARG:HG2	1:D:42:ARG:NH2	2.24	0.52
1:E:45:ASN:O	1:E:49:ILE:HG23	2.10	0.52
1:B:6:VAL:HA	1:B:37:MET:HG3	1.92	0.51
1:C:187:VAL:CG1	1:C:191:PHE:CE2	2.93	0.51
1:F:172:TRP:CZ2	1:F:424:ILE:HG12	2.45	0.51
1:D:30:GLU:HG3	1:D:61:PRO:HB2	1.93	0.51
1:E:344:GLU:HG2	1:E:346:HIS:ND1	2.25	0.51
1:A:193:ARG:HG3	1:A:249:MET:HG3	1.93	0.51
1:B:53:LYS:NZ	1:B:57:GLU:OE2	2.37	0.51
1:C:308:ARG:HH11	1:C:308:ARG:CG	2.23	0.51
1:E:344:GLU:HG2	1:E:346:HIS:CE1	2.46	0.51
1:B:177:ILE:C	1:B:178:ILE:HD12	2.35	0.51
1:A:37:MET:HE3	1:A:70:LEU:N	2.24	0.51
1:C:53:LYS:O	1:C:57:GLU:HG3	2.11	0.51
1:C:98:ARG:HD2	1:C:128:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:LYS:O	1:D:57:GLU:HG3	2.10	0.51
1:A:244:PRO:HB2	1:A:293:ILE:HG12	1.93	0.51
1:C:372:LYS:NZ	1:C:373:ASP:OD2	2.42	0.51
1:F:54:TYR:O	1:F:58:LEU:HD23	2.11	0.51
1:E:442:LYS:HE3	1:F:442:LYS:NZ	2.26	0.50
1:C:400:LEU:HD13	1:C:409:LEU:HD11	1.92	0.50
1:D:133:TYR:HB3	1:D:134:PRO:HD3	1.93	0.50
1:C:75:GLU:HB2	1:C:149:MET:CE	2.39	0.50
1:D:310:ARG:NE	3:D:1521:HOH:O	2.39	0.50
1:E:331:LYS:HD2	1:E:332:HIS:NE2	2.27	0.50
1:E:334:GLU:H	1:E:334:GLU:CD	2.18	0.50
1:C:181:CYS:SG	1:C:182:HIS:N	2.83	0.50
1:A:289:ARG:NH2	1:A:289:ARG:CG	2.65	0.50
1:E:29:ARG:NH1	1:E:31:ASP:OD1	2.45	0.50
1:D:235:GLU:CD	3:D:2149:HOH:O	2.54	0.50
1:F:424:ILE:HD11	3:F:520:HOH:O	2.12	0.50
1:D:258:ARG:NH2	3:D:549:HOH:O	2.44	0.50
1:A:310:ARG:HD3	3:A:814:HOH:O	2.11	0.49
1:E:232:ILE:HD13	1:E:258:ARG:NH1	2.27	0.49
1:C:45:ASN:O	1:C:49:ILE:HG23	2.11	0.49
1:C:24:THR:HB	1:C:27:LEU:HB2	1.94	0.49
1:B:378:LEU:HD21	1:B:413:ILE:CD1	2.42	0.49
1:E:326:LEU:HD23	1:E:327:LYS:N	2.27	0.49
1:A:400:LEU:HD13	1:A:409:LEU:HD11	1.95	0.49
1:C:98:ARG:CZ	3:C:558:HOH:O	2.60	0.49
1:D:464:ARG:NH1	1:D:468:GLU:OE2	2.46	0.49
1:E:310:ARG:NH1	1:E:311:GLU:OE1	2.45	0.49
1:E:468:GLU:OE2	3:E:2426:HOH:O	2.18	0.49
1:E:49:ILE:HD11	1:E:317:ALA:C	2.37	0.49
1:C:344:GLU:CG	1:C:346:HIS:HD1	2.26	0.49
1:D:144:GLU:OE1	1:D:147:LYS:HE2	2.12	0.49
1:B:172:TRP:CZ2	1:B:424:ILE:HG12	2.48	0.49
1:E:71:ASP:O	1:E:149:MET:HE1	2.13	0.49
1:F:193:ARG:HE	1:F:193:ARG:HA	1.76	0.49
1:B:49:ILE:HD12	1:B:317:ALA:HA	1.94	0.48
1:C:49:ILE:HD11	1:C:317:ALA:O	2.14	0.48
1:C:284:LYS:O	1:C:288:ARG:HA	2.13	0.48
1:B:310:ARG:HD3	3:B:1425:HOH:O	2.13	0.48
1:B:144:GLU:OE1	1:B:147:LYS:HE2	2.13	0.48
1:D:170:ARG:HD3	1:D:366:GLU:OE2	2.13	0.48
1:C:182:HIS:CD2	1:C:345:GLN:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:HD23	1:E:412:ARG:HG2	1.94	0.48
1:D:243:ASN:HB2	1:D:244:PRO:CD	2.44	0.48
1:B:42:ARG:HH21	1:B:45:ASN:ND2	2.12	0.48
1:C:26:GLU:OE1	1:C:26:GLU:N	2.30	0.48
1:F:33:HIS:CD2	1:F:63:LYS:HD2	2.48	0.48
1:B:37:MET:HE2	1:B:38:ASP:N	2.29	0.48
1:D:344:GLU:HG2	1:D:346:HIS:HD1	1.78	0.48
1:B:181:CYS:SG	1:B:182:HIS:N	2.87	0.48
1:C:289:ARG:HD3	1:F:462:GLU:CD	2.39	0.48
1:F:464:ARG:NE	3:F:1930:HOH:O	1.95	0.48
1:F:71:ASP:OD2	3:F:2121:HOH:O	2.20	0.47
1:A:141:GLU:OE2	3:A:776:HOH:O	2.20	0.47
1:C:356:ASN:OD1	1:C:388:SER:OG	2.15	0.47
1:A:48:TYR:CE2	1:A:52:ARG:HD2	2.49	0.47
1:A:170:ARG:HD3	1:A:366:GLU:OE2	2.14	0.47
1:D:157:GLN:HB2	1:D:177:ILE:HD11	1.96	0.47
1:A:243:ASN:HB2	1:A:244:PRO:HD2	1.96	0.47
1:C:412:ARG:NE	3:C:1570:HOH:O	2.45	0.47
1:D:137:LYS:O	1:D:141:GLU:HG3	2.14	0.47
1:D:322:GLU:O	1:D:323:ASN:CB	2.62	0.47
1:B:364:ASN:HA	1:B:380:MET:O	2.14	0.47
1:D:40:HIS:CE1	1:D:43:ARG:HG3	2.50	0.47
1:D:53:LYS:NZ	1:D:326:LEU:O	2.47	0.47
1:A:208:VAL:HG11	1:A:412:ARG:HG2	1.96	0.47
1:F:412:ARG:HD2	3:F:553:HOH:O	2.14	0.47
1:C:199:GLU:CD	3:C:2175:HOH:O	2.58	0.46
1:D:179:GLY:HA3	1:D:364:ASN:HB2	1.96	0.46
1:D:299:ARG:HB3	1:D:300:PRO:HD3	1.97	0.46
1:F:193:ARG:HG3	1:F:249:MET:HG3	1.97	0.46
1:F:304:GLU:HG3	1:F:308:ARG:HE	1.80	0.46
1:F:222:LYS:NZ	3:F:1539:HOH:O	2.46	0.46
1:A:222:LYS:CD	1:A:223:ASP:N	2.73	0.46
1:B:117:SER:O	1:B:440:ARG:NH2	2.48	0.46
1:A:301:LYS:NZ	3:A:1244:HOH:O	2.48	0.46
1:B:1:MET:HE2	1:B:3:ILE:HG13	1.97	0.46
1:B:88:ASP:OD2	1:B:90:ARG:NH1	2.49	0.46
1:C:299:ARG:HB3	1:C:300:PRO:HD3	1.97	0.46
1:D:344:GLU:HG2	1:D:346:HIS:ND1	2.31	0.46
1:C:209:ASN:O	1:C:412:ARG:NH2	2.48	0.46
1:D:439:PRO:HD2	3:D:532:HOH:O	2.15	0.46
1:F:30:GLU:OE2	1:F:63:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:TYR:OH	3:F:559:HOH:O	2.17	0.46
1:B:208:VAL:HG11	1:B:412:ARG:HG2	1.98	0.46
1:C:26:GLU:H	1:C:26:GLU:CD	2.21	0.46
1:D:326:LEU:C	1:D:327:LYS:HE3	2.40	0.46
1:A:70:LEU:HD22	1:A:74:ILE:CD1	2.46	0.46
1:A:323:ASN:C	1:A:325:HIS:H	2.23	0.46
1:C:98:ARG:HD2	1:C:128:TYR:CZ	2.51	0.46
1:D:329:THR:HB	1:D:338:LYS:HE2	1.98	0.46
1:E:219:TYR:CE2	1:E:220:ARG:HG3	2.51	0.46
1:B:320:VAL:CG2	1:B:328:ILE:HD11	2.45	0.45
1:C:301:LYS:HE2	1:C:301:LYS:HB2	1.78	0.45
1:E:464:ARG:NH2	3:E:2038:HOH:O	2.47	0.45
1:B:157:GLN:HB2	1:B:177:ILE:HD11	1.98	0.45
1:C:405:LYS:HE2	3:C:626:HOH:O	2.16	0.45
1:E:137:LYS:HE2	1:E:141:GLU:OE2	2.17	0.45
1:A:182:HIS:CE1	1:A:345:GLN:N	2.65	0.45
1:D:312:ARG:HA	1:D:315:LYS:HE3	1.97	0.45
1:E:193:ARG:HG3	1:E:249:MET:HG3	1.99	0.45
1:A:104:LYS:HB3	3:A:1043:HOH:O	2.15	0.45
1:B:335:ILE:C	1:B:337:PRO:HD3	2.42	0.45
1:D:129:VAL:O	1:D:130:LEU:HB2	2.16	0.45
1:E:293:ILE:HG12	1:E:293:ILE:O	2.16	0.45
1:F:1:MET:HE1	1:F:354:ALA:HB2	1.99	0.45
1:A:45:ASN:OD1	1:A:66:LYS:NZ	2.50	0.45
1:A:438:ASP:HA	1:A:439:PRO:HD3	1.86	0.45
1:C:37:MET:HE2	1:C:38:ASP:C	2.42	0.45
1:C:141:GLU:HG3	3:C:542:HOH:O	2.16	0.45
1:F:133:TYR:HB3	1:F:134:PRO:HD3	1.97	0.45
1:C:182:HIS:CE1	1:C:344:GLU:HG3	2.52	0.45
1:E:40:HIS:HB2	3:E:1094:HOH:O	2.16	0.45
1:E:125:THR:HG21	3:E:958:HOH:O	2.16	0.45
1:F:26:GLU:CD	3:F:829:HOH:O	2.49	0.45
1:B:318:GLU:O	1:B:322:GLU:HG2	2.17	0.45
1:E:322:GLU:OE2	1:E:322:GLU:N	2.50	0.45
1:F:193:ARG:NH2	1:F:231:TRP:HE1	2.14	0.45
1:C:331:LYS:O	1:C:333:PRO:HD3	2.17	0.44
1:E:439:PRO:HA	1:F:439:PRO:HA	1.99	0.44
1:D:38:ASP:OD1	1:D:39:VAL:N	2.49	0.44
1:F:52:ARG:O	1:F:55:VAL:HG22	2.17	0.44
1:F:420:LEU:O	1:F:424:ILE:HG13	2.18	0.44
1:B:225:TYR:N	1:B:226:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:HIS:HB2	1:C:412:ARG:HH22	1.82	0.44
1:B:202:ASP:HB3	1:B:218:ARG:HB2	2.00	0.44
1:C:29:ARG:CA	1:C:61:PRO:HG2	2.47	0.44
1:C:245:TRP:CZ3	3:C:1569:HOH:O	2.68	0.44
1:E:299:ARG:HB3	1:E:300:PRO:HD3	1.98	0.44
1:F:182:HIS:CD2	1:F:344:GLU:HG3	2.52	0.44
1:A:157:GLN:HB2	1:A:177:ILE:HD11	1.99	0.44
1:F:2:LYS:HE3	1:F:35:TYR:CD1	2.53	0.44
1:A:230:GLU:CD	1:A:234:LYS:NZ	2.75	0.44
1:B:328:ILE:H	1:B:328:ILE:CD1	2.29	0.44
1:C:219:TYR:CD2	1:C:220:ARG:HG3	2.53	0.44
1:C:233:GLU:HG2	3:C:1413:HOH:O	2.17	0.44
1:E:216:ARG:HD3	1:E:397:GLU:O	2.18	0.44
1:E:274:TRP:CD1	1:E:439:PRO:HG2	2.53	0.44
1:F:182:HIS:HD2	1:F:344:GLU:HA	1.82	0.44
1:C:11:VAL:O	1:C:15:LEU:HG	2.18	0.43
1:C:15:LEU:O	1:C:19:GLU:HG3	2.18	0.43
1:D:296:GLU:H	1:D:296:GLU:CD	2.26	0.43
1:E:56:GLU:HG3	1:E:57:GLU:N	2.30	0.43
1:C:289:ARG:CD	1:F:462:GLU:HG3	2.48	0.43
1:C:42:ARG:HA	1:C:42:ARG:NE	2.33	0.43
1:C:79:PHE:CE2	1:C:350:ILE:HG23	2.53	0.43
1:F:53:LYS:O	1:F:57:GLU:HG3	2.19	0.43
1:A:181:CYS:SG	1:A:182:HIS:N	2.92	0.43
1:C:129:VAL:O	1:C:130:LEU:HB2	2.18	0.43
1:C:243:ASN:HB2	1:C:244:PRO:CD	2.49	0.43
1:F:182:HIS:CE1	1:F:345:GLN:HB2	2.54	0.43
1:F:230:GLU:O	1:F:234:LYS:HE2	2.18	0.43
1:F:230:GLU:CD	3:F:1929:HOH:O	2.62	0.43
1:A:187:VAL:HG22	1:A:191:PHE:CZ	2.53	0.43
1:B:356:ASN:OD1	1:B:387:ASP:HB2	2.18	0.43
1:A:205:VAL:HG22	1:A:362:PHE:CE2	2.54	0.43
1:B:209:ASN:O	1:B:412:ARG:NH2	2.52	0.43
1:C:347:ILE:N	1:C:348:PRO:CD	2.82	0.43
1:C:442:LYS:NZ	3:C:1851:HOH:O	2.51	0.43
1:C:182:HIS:HE1	1:C:346:HIS:CE1	2.36	0.43
1:D:335:ILE:C	1:D:337:PRO:HD3	2.44	0.43
1:F:230:GLU:HG3	1:F:234:LYS:CE	2.48	0.43
1:B:187:VAL:HG22	1:B:191:PHE:CZ	2.54	0.43
1:E:410:TRP:HB3	1:F:414:LEU:HD11	2.01	0.43
1:A:70:LEU:HD22	1:A:74:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HG3	3:A:545:HOH:O	2.19	0.42
1:E:109:HIS:CG	1:E:450:VAL:HG22	2.55	0.42
1:A:163:PHE:CE2	1:A:208:VAL:HG22	2.54	0.42
1:A:372:LYS:NZ	1:A:372:LYS:HB3	2.34	0.42
1:A:45:ASN:O	1:A:49:ILE:HG12	2.19	0.42
1:A:222:LYS:CD	1:A:223:ASP:H	2.11	0.42
1:B:299:ARG:HB3	1:B:300:PRO:HD3	2.01	0.42
1:C:49:ILE:CD1	1:C:317:ALA:HB1	2.47	0.42
1:A:143:ALA:O	1:A:147:LYS:HG3	2.19	0.42
1:A:270:ARG:CD	1:A:294:ASP:OD2	2.62	0.42
1:A:433:GLU:O	1:A:437:ARG:HG2	2.20	0.42
1:B:193:ARG:HH12	1:B:239:TRP:HE1	1.65	0.42
1:C:225:TYR:N	1:C:226:PRO:CD	2.83	0.42
1:F:182:HIS:HE2	1:F:344:GLU:HG3	1.83	0.42
1:C:16:GLN:OE1	1:C:342:SER:HB2	2.20	0.42
1:B:464:ARG:NH1	3:B:2233:HOH:O	2.52	0.42
1:C:140:LEU:HD23	1:C:169:VAL:HG22	2.02	0.42
1:C:193:ARG:CD	3:C:1683:HOH:O	2.55	0.42
1:D:202:ASP:HB3	1:D:218:ARG:HB2	2.02	0.42
1:F:75:GLU:OE1	1:F:149:MET:HG2	2.19	0.42
1:E:49:ILE:HD11	1:E:317:ALA:CA	2.50	0.42
1:E:125:THR:O	1:E:125:THR:HG23	2.20	0.42
1:F:317:ALA:O	1:F:320:VAL:HG22	2.20	0.42
1:A:216:ARG:HD3	1:A:397:GLU:O	2.20	0.41
1:B:296:GLU:H	1:B:296:GLU:CD	2.18	0.41
1:C:318:GLU:O	1:C:321:GLN:HB3	2.20	0.41
1:E:161:PRO:HG2	1:E:164:GLU:HB2	2.02	0.41
1:F:230:GLU:HG3	1:F:234:LYS:NZ	2.35	0.41
1:A:17:LEU:O	1:A:21:ILE:HG13	2.20	0.41
1:A:323:ASN:C	1:A:325:HIS:N	2.79	0.41
1:A:364:ASN:HA	1:A:380:MET:O	2.20	0.41
1:C:263:LEU:HD12	1:C:264:PRO:HD2	2.02	0.41
1:D:14:ALA:O	1:D:18:VAL:HG23	2.21	0.41
1:E:170:ARG:HD3	1:E:366:GLU:OE2	2.21	0.41
1:F:326:LEU:HD21	1:F:331:LYS:HD2	2.01	0.41
1:B:53:LYS:HG2	1:B:328:ILE:HD13	2.02	0.41
1:C:2:LYS:HD3	1:C:77:ALA:HA	2.03	0.41
1:E:53:LYS:HG3	1:E:328:ILE:CD1	2.51	0.41
1:F:150:ALA:N	1:F:151:PRO:CD	2.83	0.41
1:A:231:TRP:CE2	1:A:235:GLU:HB2	2.55	0.41
1:C:205:VAL:HG22	1:C:362:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:CYS:SG	1:D:182:HIS:N	2.93	0.41
1:D:457:LEU:HA	1:D:458:PRO:HD3	1.91	0.41
1:A:225:TYR:N	1:A:226:PRO:CD	2.84	0.41
1:B:48:TYR:O	1:B:52:ARG:HG3	2.19	0.41
1:B:77:ALA:O	1:B:153:ALA:HB2	2.21	0.41
1:F:15:LEU:O	1:F:19:GLU:HG3	2.21	0.41
1:F:29:ARG:NH2	1:F:31:ASP:OD1	2.38	0.41
1:E:245:TRP:CZ2	1:E:293:ILE:HD12	2.55	0.41
1:A:409:LEU:O	1:A:413:ILE:CD1	2.64	0.41
1:B:1:MET:HE1	1:B:79:PHE:CD2	2.54	0.41
1:B:21:ILE:HG21	1:B:34:ILE:HD11	2.02	0.41
1:B:57:GLU:OE1	1:B:329:THR:OG1	2.29	0.41
1:C:288:ARG:HB3	1:C:289:ARG:H	1.75	0.41
1:D:57:GLU:OE1	1:D:329:THR:OG1	2.32	0.41
1:D:109:HIS:HB2	1:D:450:VAL:HG13	2.02	0.41
1:D:111:TYR:HE1	1:D:450:VAL:HG21	1.82	0.41
1:E:12:ARG:HA	1:E:12:ARG:HD2	1.95	0.41
1:E:98:ARG:NH1	3:E:568:HOH:O	2.54	0.41
1:F:457:LEU:HA	1:F:458:PRO:HD3	1.93	0.41
1:B:182:HIS:CE1	1:B:344:GLU:CA	2.95	0.41
1:C:133:TYR:HB3	1:C:134:PRO:HD3	2.03	0.40
1:C:344:GLU:HG2	1:C:346:HIS:HD1	1.86	0.40
1:E:371:LEU:HD12	1:E:380:MET:SD	2.61	0.40
1:F:129:VAL:O	1:F:130:LEU:HB2	2.19	0.40
1:F:356:ASN:OD1	1:F:387:ASP:HB2	2.21	0.40
1:F:440:ARG:HB2	3:F:1332:HOH:O	2.21	0.40
1:A:323:ASN:O	1:A:325:HIS:N	2.54	0.40
1:B:56:GLU:CD	1:B:56:GLU:C	2.90	0.40
1:B:262:MET:HE1	1:B:399:ASP:O	2.21	0.40
1:C:245:TRP:HH2	3:C:1569:HOH:O	2.02	0.40
1:D:193:ARG:HG3	1:D:249:MET:HG3	2.02	0.40
1:E:356:ASN:OD1	1:E:387:ASP:HB2	2.21	0.40
1:A:19:GLU:HG2	1:A:54:TYR:CZ	2.56	0.40
1:E:48:TYR:CD1	1:E:66:LYS:HB3	2.56	0.40
1:F:193:ARG:HA	1:F:193:ARG:NE	2.36	0.40
1:C:91:TYR:CE1	1:C:458:PRO:HB2	2.57	0.40
1:E:49:ILE:HD11	1:E:317:ALA:HB1	2.04	0.40
1:F:299:ARG:HB3	1:F:300:PRO:HD3	2.02	0.40
1:A:52:ARG:O	1:A:55:VAL:HG22	2.22	0.40
1:A:322:GLU:C	1:A:324:PRO:HD3	2.47	0.40
3:A:1917:HOH:O	1:B:439:PRO:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLU:HA	1:C:149:MET:HB3	2.04	0.40
1:C:327:LYS:HE2	1:C:330:GLU:CD	2.47	0.40
1:C:357:LYS:HA	1:C:357:LYS:HD2	1.89	0.40
1:C:387:ASP:OD1	1:C:387:ASP:C	2.65	0.40
1:D:193:ARG:NH2	1:D:239:TRP:CD1	2.90	0.40
1:D:344:GLU:HG2	1:D:346:HIS:CE1	2.56	0.40
1:F:137:LYS:O	1:F:141:GLU:HG3	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	466/477 (98%)	453 (97%)	11 (2%)	2 (0%)	30	27
1	B	467/477 (98%)	449 (96%)	18 (4%)	0	100	100
1	C	460/477 (96%)	441 (96%)	18 (4%)	1 (0%)	43	42
1	D	466/477 (98%)	452 (97%)	13 (3%)	1 (0%)	43	42
1	E	462/477 (97%)	445 (96%)	17 (4%)	0	100	100
1	F	467/477 (98%)	449 (96%)	17 (4%)	1 (0%)	43	42
All	All	2788/2862 (97%)	2689 (96%)	94 (3%)	5 (0%)	43	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	D	323	ASN
1	F	289	ARG
1	C	289	ARG
1	A	324	PRO

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	418/427 (98%)	387 (93%)	31 (7%)	13	9
1	B	419/427 (98%)	396 (94%)	23 (6%)	19	17
1	C	414/427 (97%)	390 (94%)	24 (6%)	18	15
1	D	418/427 (98%)	391 (94%)	27 (6%)	15	12
1	E	416/427 (97%)	387 (93%)	29 (7%)	14	10
1	F	419/427 (98%)	396 (94%)	23 (6%)	19	17
All	All	2504/2562 (98%)	2347 (94%)	157 (6%)	16	13

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	28	SER
1	A	29	ARG
1	A	36	LEU
1	A	37	MET
1	A	41	GLU
1	A	49	ILE
1	A	58	LEU
1	A	70	LEU
1	A	75	GLU
1	A	120	LEU
1	A	121	ASN
1	A	148	LYS
1	A	187	VAL
1	A	189	GLU
1	A	208	VAL
1	A	222	LYS
1	A	230	GLU
1	A	233	GLU
1	A	236	LEU
1	A	258	ARG
1	A	289	ARG

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Mol	Chain	Res	Type
1	A	293	ILE
1	A	296	GLU
1	A	306	LEU
1	A	321	GLN
1	A	326	LEU
1	A	327	LYS
1	A	372	LYS
1	A	412	ARG
1	A	420	LEU
1	B	28	SER
1	B	37	MET
1	B	49	ILE
1	B	56	GLU
1	B	70	LEU
1	B	120	LEU
1	B	187	VAL
1	B	208	VAL
1	B	220	ARG
1	B	236	LEU
1	B	258	ARG
1	B	296	GLU
1	B	308	ARG
1	B	315	LYS
1	B	318	GLU
1	B	321	GLN
1	B	338	LYS
1	B	344	GLU
1	B	357	LYS
1	B	416	THR
1	B	420	LEU
1	B	424	ILE
1	B	440	ARG
1	C	17	LEU
1	C	36	LEU
1	C	37	MET
1	C	49	ILE
1	C	70	LEU
1	C	120	LEU
1	C	121	ASN
1	C	130	LEU
1	C	178	ILE
1	C	181	CYS

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Mol	Chain	Res	Type
1	C	187	VAL
1	C	189	GLU
1	C	208	VAL
1	C	220	ARG
1	C	236	LEU
1	C	293	ILE
1	C	296	GLU
1	C	306	LEU
1	C	308	ARG
1	C	320	VAL
1	C	329	THR
1	C	331	LYS
1	C	340	ARG
1	C	357	LYS
1	D	37	MET
1	D	41	GLU
1	D	42	ARG
1	D	58	LEU
1	D	70	LEU
1	D	120	LEU
1	D	121	ASN
1	D	130	LEU
1	D	181	CYS
1	D	187	VAL
1	D	199	GLU
1	D	208	VAL
1	D	222	LYS
1	D	230	GLU
1	D	233	GLU
1	D	236	LEU
1	D	258	ARG
1	D	281	GLU
1	D	296	GLU
1	D	308	ARG
1	D	326	LEU
1	D	327	LYS
1	D	413	ILE
1	D	420	LEU
1	D	440	ARG
1	D	450	VAL
1	D	461	GLU
1	E	1	MET

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Mol	Chain	Res	Type
1	E	17	LEU
1	E	30	GLU
1	E	36	LEU
1	E	37	MET
1	E	49	ILE
1	E	56	GLU
1	E	58	LEU
1	E	70	LEU
1	E	102	VAL
1	E	130	LEU
1	E	182	HIS
1	E	208	VAL
1	E	220	ARG
1	E	233	GLU
1	E	234	LYS
1	E	236	LEU
1	E	258	ARG
1	E	288	ARG
1	E	293	ILE
1	E	296	GLU
1	E	306	LEU
1	E	331	LYS
1	E	334	GLU
1	E	344	GLU
1	E	420	LEU
1	E	440	ARG
1	E	461	GLU
1	E	465	ARG
1	F	25	ASP
1	F	37	MET
1	F	41	GLU
1	F	49	ILE
1	F	52	ARG
1	F	56	GLU
1	F	59	ASN
1	F	70	LEU
1	F	130	LEU
1	F	149	MET
1	F	181	CYS
1	F	182	HIS
1	F	208	VAL
1	F	220	ARG

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Mol	Chain	Res	Type
1	F	236	LEU
1	F	308	ARG
1	F	321	GLN
1	F	326	LEU
1	F	340	ARG
1	F	344	GLU
1	F	420	LEU
1	F	424	ILE
1	F	440	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	215	ASN
1	B	215	ASN
1	C	176	ASN
1	C	215	ASN
1	C	392	HIS
1	D	33	HIS
1	D	332	HIS
1	E	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/477 (98%)	-1.54	0 100 100	15, 26, 50, 72	0
1	B	469/477 (98%)	-1.51	0 100 100	14, 28, 56, 69	0
1	C	464/477 (97%)	-1.46	0 100 100	15, 29, 60, 74	0
1	D	468/477 (98%)	-1.53	0 100 100	14, 27, 53, 71	0
1	E	466/477 (97%)	-1.54	0 100 100	14, 26, 52, 74	0
1	F	469/477 (98%)	-1.50	0 100 100	15, 29, 57, 80	0
All	All	2804/2862 (97%)	-1.52	0 100 100	14, 28, 57, 80	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	601	1/1	0.99	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	602	1/1	1.00	0.04	48,48,48,48	0
2	MN	C	500	1/1	1.00	0.03	51,51,51,51	0
2	MN	D	600	1/1	1.00	0.04	58,58,58,58	0
2	MN	E	600	1/1	1.00	0.05	51,51,51,51	0
2	MN	F	600	1/1	1.00	0.03	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.