



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2016 – 05:12 PM EDT

PDB ID : 5FSW
Title : RNA dependent RNA polymerase QDE-1 from Thielavia terrestris
Authors : Qian, X.; Hamid, F.M.; El Sahili, A.; Darwis, D.A.; Wong, Y.H.; Bhushan, S.;
Makeyev, E.V.; Lescar, J.
Deposited on : 2016-01-08
Resolution : 3.19 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

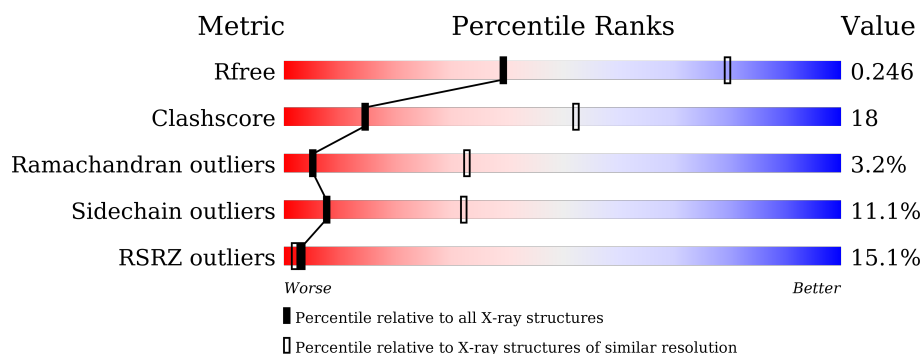
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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.

Mol	Chain	Length	Quality of chain
1	A	1034	<div> <div>4%</div> <div> <div>47%</div> <div>34%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	1034	<div> <div>10%</div> <div> <div>58%</div> <div>27%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	1034	<div> <div>18%</div> <div> <div>62%</div> <div>22%</div> <div>5%</div> <div>11%</div> </div> </div>
1	D	1034	<div> <div>22%</div> <div> <div>60%</div> <div>25%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28130 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 RNA DEPENDENT RNA POLYMERASE QDE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7358	4679	1307	1335	37			
1	B	922	Total	C	N	O	S	0	0	0
			6924	4462	1186	1244	32			
1	C	922	Total	C	N	O	S	0	0	0
			6924	4462	1186	1244	32			
1	D	922	Total	C	N	O	S	0	0	0
			6924	4462	1186	1244	32			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP G2R911
A	2	GLY	-	EXPRESSION TAG	UNP G2R911
A	3	HIS	-	EXPRESSION TAG	UNP G2R911
A	4	HIS	-	EXPRESSION TAG	UNP G2R911
A	5	HIS	-	EXPRESSION TAG	UNP G2R911
A	6	HIS	-	EXPRESSION TAG	UNP G2R911
A	7	HIS	-	EXPRESSION TAG	UNP G2R911
A	8	HIS	-	EXPRESSION TAG	UNP G2R911
A	9	SER	-	EXPRESSION TAG	UNP G2R911
A	10	SER	-	EXPRESSION TAG	UNP G2R911
A	11	GLY	-	EXPRESSION TAG	UNP G2R911
A	12	VAL	-	EXPRESSION TAG	UNP G2R911
A	13	ASP	-	EXPRESSION TAG	UNP G2R911
A	14	LEU	-	EXPRESSION TAG	UNP G2R911
A	15	GLY	-	EXPRESSION TAG	UNP G2R911
A	16	THR	-	EXPRESSION TAG	UNP G2R911
A	17	GLU	-	EXPRESSION TAG	UNP G2R911
A	18	ASN	-	EXPRESSION TAG	UNP G2R911
A	19	LEU	-	EXPRESSION TAG	UNP G2R911
A	20	TYR	-	EXPRESSION TAG	UNP G2R911
A	21	PHE	-	EXPRESSION TAG	UNP G2R911

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLN	-	EXPRESSION TAG	UNP G2R911
A	23	SER	-	EXPRESSION TAG	UNP G2R911
A	24	MET	-	EXPRESSION TAG	UNP G2R911
B	1	MET	-	EXPRESSION TAG	UNP G2R911
B	2	GLY	-	EXPRESSION TAG	UNP G2R911
B	3	HIS	-	EXPRESSION TAG	UNP G2R911
B	4	HIS	-	EXPRESSION TAG	UNP G2R911
B	5	HIS	-	EXPRESSION TAG	UNP G2R911
B	6	HIS	-	EXPRESSION TAG	UNP G2R911
B	7	HIS	-	EXPRESSION TAG	UNP G2R911
B	8	HIS	-	EXPRESSION TAG	UNP G2R911
B	9	SER	-	EXPRESSION TAG	UNP G2R911
B	10	SER	-	EXPRESSION TAG	UNP G2R911
B	11	GLY	-	EXPRESSION TAG	UNP G2R911
B	12	VAL	-	EXPRESSION TAG	UNP G2R911
B	13	ASP	-	EXPRESSION TAG	UNP G2R911
B	14	LEU	-	EXPRESSION TAG	UNP G2R911
B	15	GLY	-	EXPRESSION TAG	UNP G2R911
B	16	THR	-	EXPRESSION TAG	UNP G2R911
B	17	GLU	-	EXPRESSION TAG	UNP G2R911
B	18	ASN	-	EXPRESSION TAG	UNP G2R911
B	19	LEU	-	EXPRESSION TAG	UNP G2R911
B	20	TYR	-	EXPRESSION TAG	UNP G2R911
B	21	PHE	-	EXPRESSION TAG	UNP G2R911
B	22	GLN	-	EXPRESSION TAG	UNP G2R911
B	23	SER	-	EXPRESSION TAG	UNP G2R911
B	24	MET	-	EXPRESSION TAG	UNP G2R911
C	1	MET	-	EXPRESSION TAG	UNP G2R911
C	2	GLY	-	EXPRESSION TAG	UNP G2R911
C	3	HIS	-	EXPRESSION TAG	UNP G2R911
C	4	HIS	-	EXPRESSION TAG	UNP G2R911
C	5	HIS	-	EXPRESSION TAG	UNP G2R911
C	6	HIS	-	EXPRESSION TAG	UNP G2R911
C	7	HIS	-	EXPRESSION TAG	UNP G2R911
C	8	HIS	-	EXPRESSION TAG	UNP G2R911
C	9	SER	-	EXPRESSION TAG	UNP G2R911
C	10	SER	-	EXPRESSION TAG	UNP G2R911
C	11	GLY	-	EXPRESSION TAG	UNP G2R911
C	12	VAL	-	EXPRESSION TAG	UNP G2R911
C	13	ASP	-	EXPRESSION TAG	UNP G2R911
C	14	LEU	-	EXPRESSION TAG	UNP G2R911
C	15	GLY	-	EXPRESSION TAG	UNP G2R911

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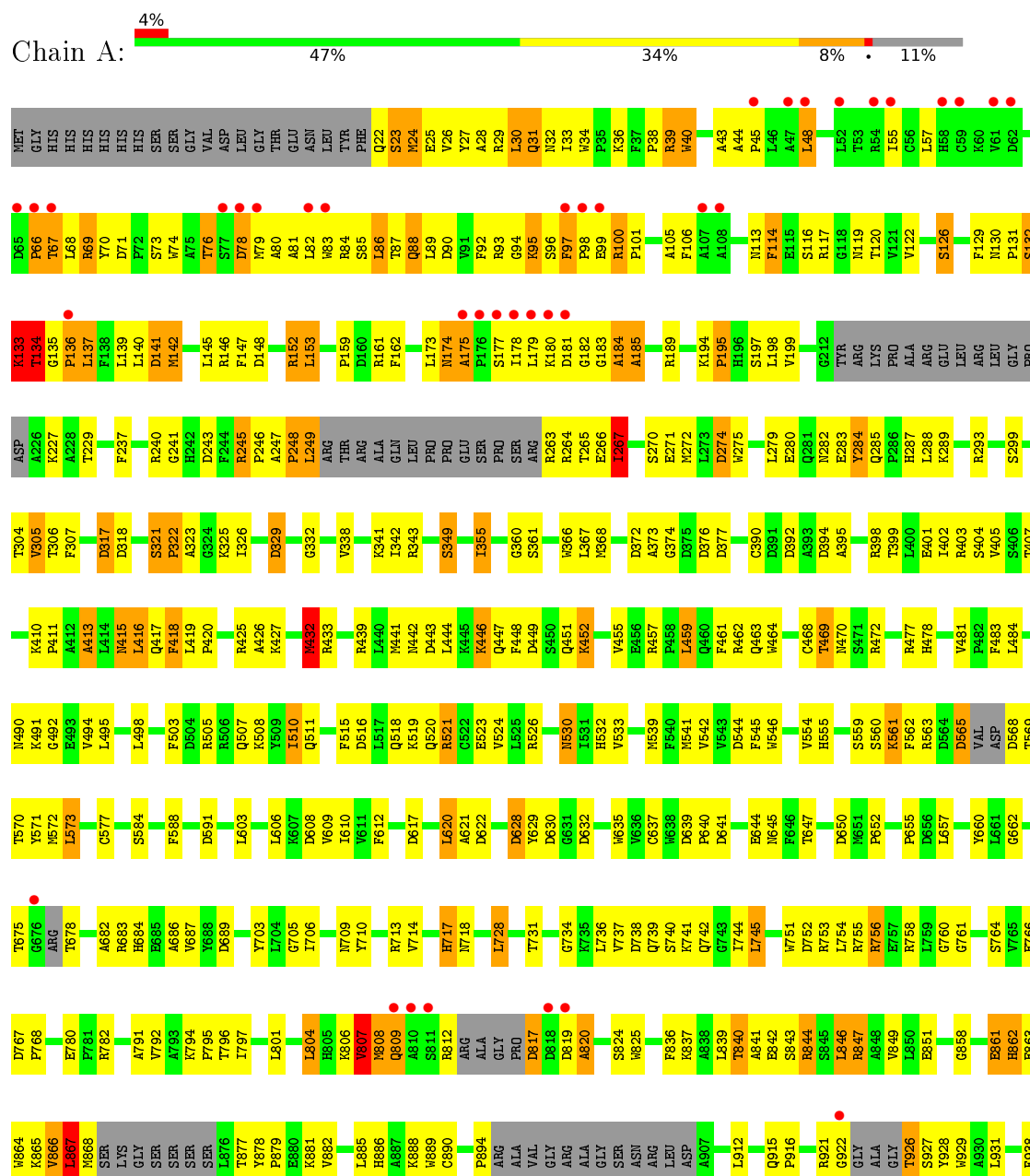
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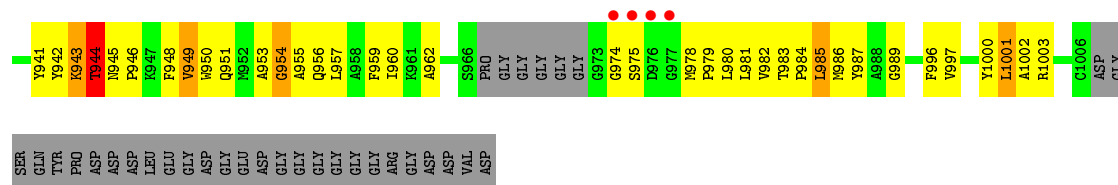
Chain	Residue	Modelled	Actual	Comment	Reference
C	16	THR	-	EXPRESSION TAG	UNP G2R911
C	17	GLU	-	EXPRESSION TAG	UNP G2R911
C	18	ASN	-	EXPRESSION TAG	UNP G2R911
C	19	LEU	-	EXPRESSION TAG	UNP G2R911
C	20	TYR	-	EXPRESSION TAG	UNP G2R911
C	21	PHE	-	EXPRESSION TAG	UNP G2R911
C	22	GLN	-	EXPRESSION TAG	UNP G2R911
C	23	SER	-	EXPRESSION TAG	UNP G2R911
C	24	MET	-	EXPRESSION TAG	UNP G2R911
D	1	MET	-	EXPRESSION TAG	UNP G2R911
D	2	GLY	-	EXPRESSION TAG	UNP G2R911
D	3	HIS	-	EXPRESSION TAG	UNP G2R911
D	4	HIS	-	EXPRESSION TAG	UNP G2R911
D	5	HIS	-	EXPRESSION TAG	UNP G2R911
D	6	HIS	-	EXPRESSION TAG	UNP G2R911
D	7	HIS	-	EXPRESSION TAG	UNP G2R911
D	8	HIS	-	EXPRESSION TAG	UNP G2R911
D	9	SER	-	EXPRESSION TAG	UNP G2R911
D	10	SER	-	EXPRESSION TAG	UNP G2R911
D	11	GLY	-	EXPRESSION TAG	UNP G2R911
D	12	VAL	-	EXPRESSION TAG	UNP G2R911
D	13	ASP	-	EXPRESSION TAG	UNP G2R911
D	14	LEU	-	EXPRESSION TAG	UNP G2R911
D	15	GLY	-	EXPRESSION TAG	UNP G2R911
D	16	THR	-	EXPRESSION TAG	UNP G2R911
D	17	GLU	-	EXPRESSION TAG	UNP G2R911
D	18	ASN	-	EXPRESSION TAG	UNP G2R911
D	19	LEU	-	EXPRESSION TAG	UNP G2R911
D	20	TYR	-	EXPRESSION TAG	UNP G2R911
D	21	PHE	-	EXPRESSION TAG	UNP G2R911
D	22	GLN	-	EXPRESSION TAG	UNP G2R911
D	23	SER	-	EXPRESSION TAG	UNP G2R911
D	24	MET	-	EXPRESSION TAG	UNP G2R911

3 Residue-property plots

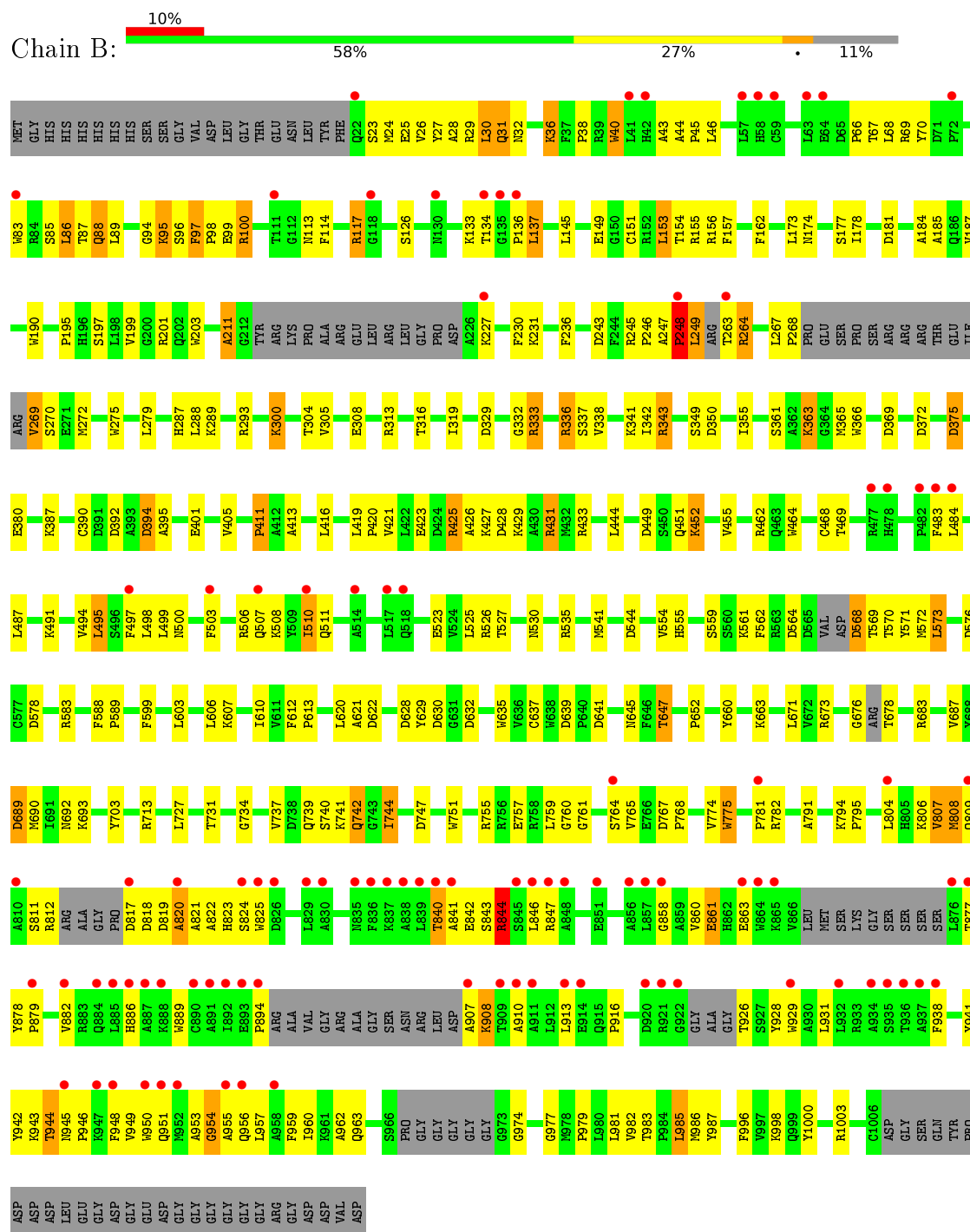
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1

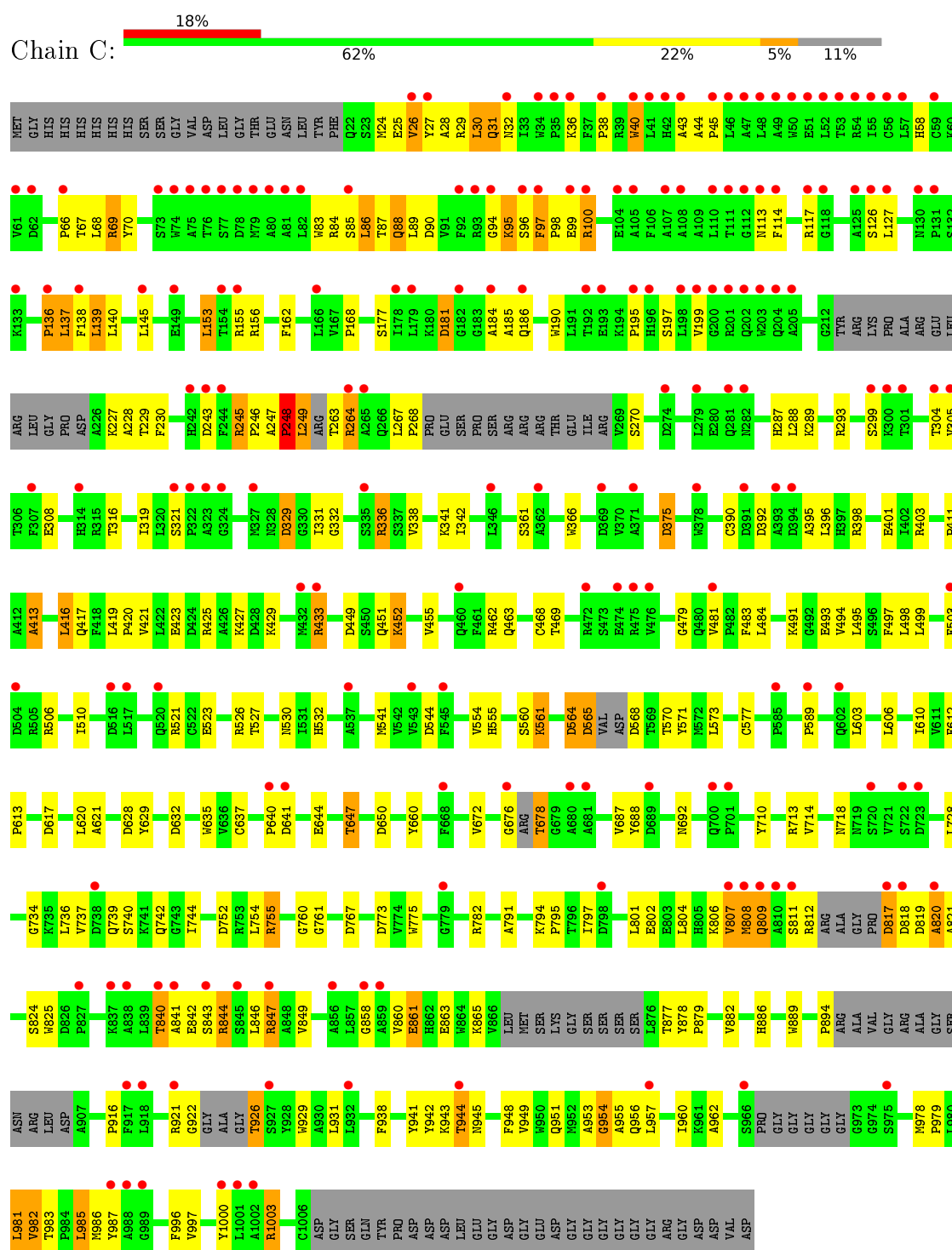




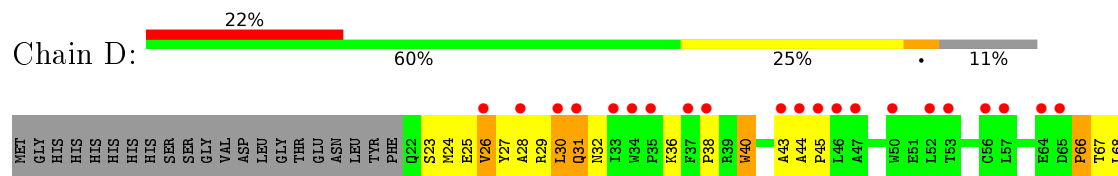
● Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



● Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



- Molecule 1: RNA DEPENDENT RNA POLYMERASE QDE-1



ASP	K943	P879	PRO	I618	T527	V455	R343	L249	T154	R69
ASP	T944	V882	D817	P619	M530	Q460	D344	ARG	R155	Y70
ASP	N945	R883	D818	A620	I531	Q463	D350	R251	F162	D71
LEU	P946	Q884	D819	A621	H532	Q464	D353	R252	P168	P72
GLY	K947	L885	A820	K623	B535	V465	S361	A253	Q254	S73
GLY	F948	L886	A821	D628	B538	V466	S362	Q254	L255	W74
ASP	V949	A887	A822	Y629	Y538	V467	K363	L255	A175	A75
ASP	W950	K888	A823	G631	M539	V469	S366	P256	S77	T76
GLU	Q951	W889	S824	G633	M541	Q470	D369	PRO	P170	D78
ASP	M952	W890	W825	D632	M544	S471	K366	GLU	A175	D78
GLY	A953	P893	D826	W633	D544	R472	W366	SER	P176	W83
GLY	G954	R894	P827	W634	D544	R473	D372	PRO	S177	R84
GLY	A955	ARG	D828	A634	V554	R476	D375	ARG	L178	R84
GLY	Q956	ALA	L829	W635	H555	Q477	D390	ARG	L179	S85
GLY	L957	VAL	F833	W636	F558	H478	D391	ARG	K180	S85
GLY	A958	GLY	E834	W637	S559	Q479	D392	ARG	L181	L86
ARG	F959	GLY	N835	W638	S560	Q480	A393	ARG	G182	T87
ARG	I960	ALA	F836	T644	S561	V481	D394	ARG	G183	Q88
GLY	I961	ALA	F837	T645	K561	V482	D394	ARG	G184	L89
ASP	K961	GLY	F838	T646	D564	Q483	D394	ARG	A184	D90
ASP	A962	GLY	A837	T647	VAL	P488	D394	ARG	A185	V91
VAL	Q963	SER	A838	T647	D568	E489	D394	ARG	Q186	F92
ASP	S966	ASN	L839	T647	L574	N490	D394	ARG	V187	R93
		ARG	T840	T647	D576	V492	D394	ARG	W190	G94
		LEU	A841	T647	D577	Q493	D394	ARG	P195	S96
		ASP	E842	T647	D578	L498	D394	ARG	P195	S97
		GLY	S843	T647	D579	M500	D394	ARG	P195	S97
		GLY	R844	T647	D579	S501	D394	ARG	P195	S97
		GLY	S845	T647	D579	S502	D394	ARG	P195	S97
		GLY	L846	T647	D579	S503	D394	ARG	P195	S97
		GLY	R847	T647	D579	S504	D394	ARG	P195	S97
		GLY	A848	T647	D579	S505	D394	ARG	P195	S97
		GLY	R849	T647	D579	S506	D394	ARG	P195	S97
		GLY	L850	T647	D579	S507	D394	ARG	P195	S97
		GLY	E851	T647	D579	S508	D394	ARG	P195	S97
		GLY	A852	T647	D579	S509	D394	ARG	P195	S97
		GLY	R855	T647	D579	S510	D394	ARG	P195	S97
		GLY	A856	T647	D579	S511	D394	ARG	P195	S97
		GLY	L857	T647	D579	S512	D394	ARG	P195	S97
		GLY	G858	T647	D579	S513	D394	ARG	P195	S97
		GLY	A859	T647	D579	S514	D394	ARG	P195	S97
		GLY	W860	T647	D579	S515	D394	ARG	P195	S97
		GLY	E861	T647	D579	S516	D394	ARG	P195	S97
		GLY	H862	T647	D579	S517	D394	ARG	P195	S97
		GLY	E863	T647	D579	S518	D394	ARG	P195	S97
		GLY	W864	T647	D579	S519	D394	ARG	P195	S97
		GLY	R865	T647	D579	S520	D394	ARG	P195	S97
		GLY	W866	T647	D579	S521	D394	ARG	P195	S97
		GLY	LEU	T647	D579	S522	D394	ARG	P195	S97
		GLY	MET	T647	D579	S523	D394	ARG	P195	S97
		GLY	SER	T647	D579	S524	D394	ARG	P195	S97
		GLY	LYS	T647	D579	S525	D394	ARG	P195	S97
		GLY	GLY	T647	D579	S526	D394	ARG	P195	S97
		GLY	SER	T647	D579	S527	D394	ARG	P195	S97
		GLY	SER	T647	D579	S528	D394	ARG	P195	S97
		GLY	SER	T647	D579	S529	D394	ARG	P195	S97
		GLY	SER	T647	D579	S530	D394	ARG	P195	S97
		GLY	SER	T647	D579	S531	D394	ARG	P195	S97
		GLY	SER	T647	D579	S532	D394	ARG	P195	S97
		GLY	SER	T647	D579	S533	D394	ARG	P195	S97
		GLY	SER	T647	D579	S534	D394	ARG	P195	S97
		GLY	SER	T647	D579	S535	D394	ARG	P195	S97
		GLY	SER	T647	D579	S536	D394	ARG	P195	S97
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		GLY	SER	T647	D579	S540	D394	ARG	P195	S97
		GLY	SER	T647	D579	S541	D394	ARG	P195	S97
		GLY	SER	T647	D579	S542	D394	ARG	P195	S97
		GLY	SER	T647	D579	S543	D394	ARG	P195	S97
		GLY	SER	T647	D579	S544	D394	ARG	P195	S97
		GLY	SER	T647	D579	S545	D394	ARG	P195	S97
		GLY	SER	T647	D579	S546	D394	ARG	P195	S97
		GLY	SER	T647	D579	S547	D394	ARG	P195	S97
		GLY	SER	T647	D579	S548	D394	ARG	P195	S97
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		GLY	SER	T647	D579	S550	D394	ARG	P195	S97
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		GLY	SER	T647	D579	S552	D394	ARG	P195	S97
		GLY	SER	T647	D579	S553	D394	ARG	P195	S97
		GLY	SER	T647	D579	S554	D394	ARG	P195	S97
		GLY	SER	T647	D579	S555	D394	ARG	P195	S97
		GLY	SER	T647	D579	S556	D394	ARG	P195	S97
		GLY	SER	T647	D579	S557	D394	ARG	P195	S97
		GLY	SER	T647	D579	S558	D394	ARG	P195	S97
		GLY	SER	T647	D579	S559	D394	ARG	P195	S97
		GLY	SER	T647	D579	S560	D394	ARG	P195	S97
		GLY	SER	T647	D579	S561	D394	ARG	P195	S97
		GLY	SER	T647	D579	S562	D394	ARG	P195	S97
		GLY	SER	T647	D579	S563	D394	ARG	P195	S97
		GLY	SER	T647	D579	S564	D394	ARG	P195	S97
		GLY	SER	T647	D579	S565	D394	ARG	P195	S97
		GLY	SER	T647	D579	S566	D394	ARG	P195	S97
		GLY	SER	T647	D579	S567	D394	ARG	P195	S97
		GLY	SER	T647	D579	S568	D394	ARG	P195	S97
		GLY	SER	T647	D579	S569	D394	ARG	P195	S97
		GLY	SER	T647	D579	S570	D394	ARG	P195	S97
		GLY	SER	T647	D579	S571	D394	ARG	P195	S97
		GLY	SER	T647	D579	S572	D394	ARG	P195	S97
		GLY	SER	T647	D579	S573	D394	ARG	P195	S97
		GLY	SER	T647	D579	S574	D394	ARG	P195	S97
		GLY	SER	T647	D579	S575	D394	ARG	P195	S97
		GLY	SER	T647	D579	S576	D394	ARG	P195	S97
		GLY	SER	T647	D579	S577	D394	ARG	P195	S97
		GLY	SER	T647	D579	S578	D394	ARG	P195	S97
		GLY	SER	T647	D579	S579	D394	ARG	P195	S97
		GLY	SER	T647	D579	S580	D394	ARG	P195	S97
		GLY	SER	T647	D579	S581	D394	ARG	P195	S97
		GLY	SER	T647	D579	S582	D394	ARG	P195	S97
		GLY	SER	T647	D579	S583	D394	ARG	P195	S97
		GLY	SER	T647	D579	S584	D394	ARG	P195	S97
		GLY	SER	T647	D579	S585	D394	ARG	P195	S97
		GLY	SER	T647	D579	S586	D394	ARG	P195	S97
		GLY	SER	T647	D579	S587	D394	ARG	P195	S97
		GLY	SER	T647	D579	S588	D394	ARG	P195	S97
		GLY	SER	T647	D579	S589	D394	ARG	P195	S97
		GLY	SER	T647	D579	S590	D394	ARG	P195	S97
		GLY	SER	T647	D579	S591	D394	ARG	P195	S97
		GLY	SER	T647	D579	S592	D394	ARG	P195	S97
		GLY	SER	T647	D579	S593	D394	ARG	P195	S97
		GLY	SER	T647	D579	S594	D394	ARG	P195	S97
		GLY	SER	T647	D579	S595	D394	ARG	P195	S97
		GLY	SER	T647	D579	S596	D394	ARG	P195	S97
		GLY	SER	T647	D579	S597	D394	ARG	P195	S97
		GLY	SER	T647	D579	S598	D394	ARG	P195	S97
		GLY	SER	T647	D579	S599	D394	ARG	P195	S97
		GLY	SER	T647	D579	S600	D394	ARG	P195	S97
		GLY	SER	T647	D579	S601	D394	ARG	P195	S97
		GLY	SER	T647	D579	S602	D394	ARG	P195	S97
		GLY	SER	T647	D579	S603	D394	ARG	P195	S97
		GLY	SER	T647	D579	S604	D394	ARG	P195	S97
		GLY	SER	T647	D579	S605	D394	ARG	P195	S97
		GLY	SER	T647	D579	S606	D394	ARG	P195	S97
		GLY	SER	T647	D579	S607	D394	ARG	P195	S97
		GLY	SER	T647	D579	S608	D394	ARG	P195	S97
		GLY	SER	T647	D579	S609	D394	ARG	P195	S97
		GLY	SER	T647	D579	S610	D394	ARG	P195	S97
		GLY	SER	T647	D579	S611	D394	ARG	P195	S97
		GLY	SER	T647	D579	S612	D394	ARG	P195	S97
		GLY	SER	T647	D579	S613	D394	ARG	P195	S97
		GLY	SER	T647	D579	S614	D394	ARG	P195	S97
		GLY	SER	T647	D579	S615	D394	ARG	P195	S97
		GLY	SER	T647	D579	S616	D394	ARG	P195	S97
		GLY	SER	T647	D579	S617	D394	ARG	P195	S97
		GLY	SER	T647	D579	S618	D394	ARG	P195	S97
		GLY	SER	T647	D579	S619	D394	ARG	P195	S97
		GLY	SER	T647	D579	S620	D394	ARG	P195	S97
		GLY	SER	T647	D579	S621	D394	ARG	P195	S97
		GLY	SER	T647	D579	S622	D394	ARG	P195	S97
		GLY	SER	T647	D5					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.23Å 165.95Å 173.89Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	48.91 – 3.19 48.91 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-3.19) 99.7 (48.91-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.98 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.213 , 0.251 0.209 , 0.246	Depositor DCC
R_{free} test set	3829 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k 0.009 for -h,-l,-k 0.052 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28130	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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	0.92	8/7528 (0.1%)	1.07	25/10177 (0.2%)
1	B	0.82	6/7063 (0.1%)	0.97	20/9494 (0.2%)
1	C	0.56	0/7063	0.85	6/9494 (0.1%)
1	D	0.56	0/7062	0.82	5/9491 (0.1%)
All	All	0.74	14/28716 (0.0%)	0.93	56/38656 (0.1%)

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	8
1	B	0	1
1	D	0	1
All	All	0	10

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	GLU	CD-OE1	6.83	1.33	1.25
1	B	308	GLU	CG-CD	6.73	1.62	1.51
1	A	284	TYR	CD1-CE1	-6.49	1.29	1.39
1	A	401	GLU	CD-OE1	6.43	1.32	1.25
1	A	349	SER	CB-OG	6.19	1.50	1.42
1	A	546	TRP	CB-CG	6.06	1.61	1.50
1	B	308	GLU	CD-OE2	5.96	1.32	1.25
1	A	283	GLU	CD-OE2	5.92	1.32	1.25
1	B	632	ASP	CB-CG	5.78	1.63	1.51
1	A	571	TYR	CD1-CE1	-5.64	1.30	1.39
1	B	375	ASP	CB-CG	5.36	1.63	1.51
1	B	757	GLU	CD-OE1	-5.20	1.20	1.25
1	A	133	LYS	N-CA	5.15	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	PHE	CB-CG	-5.09	1.42	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	632	ASP	CB-CG-OD2	-13.18	106.44	118.30
1	A	425	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	B	632	ASP	CB-CG-OD1	11.51	128.66	118.30
1	B	333	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	A	650	ASP	CB-CG-OD1	8.67	126.10	118.30
1	B	583	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	630	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	583	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	376	ASP	CB-CG-OD1	-7.64	111.42	118.30
1	A	355	ILE	CG1-CB-CG2	-7.52	94.86	111.40
1	B	622	ASP	CB-CG-OD1	7.40	124.96	118.30
1	A	565	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	331	ILE	CB-CA-C	-7.03	97.54	111.60
1	B	336	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	755	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	376	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	628	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	300	LYS	CA-CB-CG	6.73	128.20	113.40
1	A	571	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	A	321	SER	C-N-CA	-6.42	95.06	122.00
1	C	336	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	425	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	535	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	152	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	921	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	535	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	578	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	B	576	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	B	571	TYR	CA-CB-CG	5.85	124.51	113.40
1	B	630	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	305	VAL	CG1-CB-CG2	-5.84	101.55	110.90
1	A	57	LEU	CA-CB-CG	5.72	128.47	115.30
1	A	377	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	744	ILE	CB-CA-C	-5.69	100.22	111.60
1	A	274	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	641	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	630	ASP	CB-CG-OD1	5.58	123.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	943	LYS	C-N-CA	5.55	135.57	121.70
1	A	432	MET	CG-SD-CE	-5.54	91.33	100.20
1	D	632	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	510	ILE	CG1-CB-CG2	-5.46	99.39	111.40
1	B	313	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	641	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	C	713	ARG	CG-CD-NE	5.39	123.11	111.80
1	B	343	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	571	TYR	CB-CA-C	-5.38	99.65	110.40
1	C	767	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	630	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	944	THR	N-CA-CB	5.34	120.44	110.30
1	B	279	LEU	CB-CA-C	-5.31	100.11	110.20
1	C	433	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	329	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	425	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	578	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	728	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	A	846	LEU	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	SER	Peptide
1	A	174	ASN	Peptide
1	A	322	PRO	Peptide
1	A	373	ALA	Peptide
1	A	426	ALA	Peptide
1	A	68	LEU	Peptide
1	A	76	THR	Peptide
1	A	867	LEU	Peptide
1	B	568	ASP	Peptide
1	D	69	ARG	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	7358	0	7279	444	0
1	B	6924	0	6423	216	0
1	C	6924	0	6423	181	0
1	D	6924	0	6422	199	0
All	All	28130	0	26547	981	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 18.

All (981) 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:321:SER:O	1:A:323:ALA:HA	1.24	1.30
1:A:943:LYS:HB2	1:A:944:THR:OG1	1.16	1.25
1:A:321:SER:O	1:A:323:ALA:CA	1.86	1.23
1:A:133:LYS:CA	1:A:135:GLY:H	1.56	1.17
1:A:355:ILE:CD1	1:A:405:VAL:HG12	1.75	1.16
1:A:86:LEU:HB3	1:A:87:THR:OG1	1.47	1.15
1:A:133:LYS:HA	1:A:135:GLY:N	1.63	1.13
1:A:80:ALA:O	1:A:84:ARG:HG3	1.50	1.09
1:A:87:THR:HG22	1:A:92:PHE:HB3	1.13	1.07
1:A:280:GLU:OE2	1:A:683:ARG:HD3	1.54	1.06
1:B:511:GLN:NE2	1:B:808:MET:O	1.89	1.06
1:A:462:ARG:HD3	1:B:986:MET:HE1	1.34	1.05
1:A:819:ASP:HA	1:A:820:ALA:O	1.56	1.03
1:A:943:LYS:CB	1:A:944:THR:OG1	2.07	1.02
1:A:355:ILE:HD13	1:A:405:VAL:HG12	1.39	1.01
1:D:819:ASP:HA	1:D:820:ALA:O	1.62	1.00
1:B:943:LYS:HB2	1:B:944:THR:CB	1.92	0.99
1:A:280:GLU:OE2	1:A:683:ARG:CD	2.08	0.99
1:D:943:LYS:HB2	1:D:944:THR:CB	1.93	0.98
1:B:819:ASP:HA	1:B:820:ALA:O	1.62	0.97
1:D:279:LEU:HB2	1:D:683:ARG:CZ	1.95	0.97
1:A:133:LYS:HA	1:A:135:GLY:H	0.80	0.97
1:C:943:LYS:HB2	1:C:944:THR:CB	1.93	0.96
1:C:819:ASP:HA	1:C:820:ALA:O	1.66	0.94
1:A:173:LEU:HD11	1:A:180:LYS:HG2	1.47	0.94
1:A:87:THR:HG22	1:A:92:PHE:CB	1.97	0.93
1:B:23:SER:CB	1:B:24:MET:HA	1.98	0.93
1:A:31:GLN:HB3	1:A:32:ASN:HB3	1.52	0.91
1:A:321:SER:C	1:A:323:ALA:HA	1.90	0.90
1:C:806:LYS:HB3	1:C:807:VAL:CB	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:HA	1:B:88:GLN:O	1.73	0.89
1:D:846:LEU:H	1:D:847:ARG:CB	1.85	0.89
1:A:745:LEU:HD23	1:A:745:LEU:O	1.73	0.88
1:A:839:LEU:H	1:A:840:THR:HG22	1.35	0.88
1:A:843:SER:OG	1:A:847:ARG:HB2	1.72	0.88
1:C:846:LEU:H	1:C:847:ARG:CB	1.86	0.87
1:A:23:SER:OG	1:A:26:VAL:O	1.91	0.87
1:A:943:LYS:HB2	1:A:944:THR:CB	2.04	0.87
1:D:87:THR:HA	1:D:88:GLN:O	1.76	0.86
1:B:846:LEU:H	1:B:847:ARG:CB	1.89	0.85
1:A:462:ARG:HD3	1:B:986:MET:CE	2.07	0.85
1:A:804:LEU:HA	1:A:807:VAL:HG11	1.60	0.84
1:C:87:THR:HA	1:C:88:GLN:O	1.78	0.83
1:A:804:LEU:CA	1:A:807:VAL:HG11	2.08	0.83
1:D:23:SER:CB	1:D:24:MET:HA	2.10	0.82
1:A:979:PRO:O	1:B:959:PHE:CE1	2.33	0.82
1:A:703:TYR:HA	1:A:706:ILE:CG2	2.09	0.82
1:D:846:LEU:N	1:D:847:ARG:CB	2.41	0.82
1:B:31:GLN:HB3	1:B:32:ASN:HB3	1.61	0.82
1:A:129:PHE:CZ	1:A:179:LEU:CD1	2.63	0.82
1:A:263:ARG:HB2	1:A:264:ARG:HA	1.62	0.81
1:A:87:THR:HA	1:A:88:GLN:O	1.79	0.81
1:A:367:LEU:HD21	1:A:545:PHE:CE1	2.16	0.81
1:A:87:THR:CG2	1:A:92:PHE:HB3	2.05	0.81
1:C:95:LYS:H	1:C:96:SER:HA	1.46	0.80
1:B:846:LEU:N	1:B:847:ARG:CB	2.44	0.80
1:A:321:SER:HB3	1:A:323:ALA:C	2.01	0.80
1:C:846:LEU:N	1:C:847:ARG:CB	2.44	0.80
1:A:705:GLY:O	1:A:709:ASN:ND2	2.15	0.80
1:A:710:TYR:O	1:A:714:VAL:HG23	1.81	0.79
1:A:979:PRO:HB3	1:B:981:LEU:HD22	1.64	0.79
1:A:181:ASP:OD1	1:A:182:GLY:N	2.16	0.79
1:A:804:LEU:C	1:A:807:VAL:HG11	2.02	0.79
1:C:1000:TYR:CE2	1:D:985:LEU:HD23	2.17	0.79
1:A:33:ILE:HG22	1:A:140:LEU:HD11	1.65	0.79
1:A:280:GLU:OE2	1:A:683:ARG:NE	2.16	0.79
1:A:299:SER:OG	1:A:403:ARG:NH1	2.15	0.79
1:A:912:LEU:O	1:A:915:GLN:CG	2.30	0.78
1:A:662:GLY:O	1:A:745:LEU:HB3	1.82	0.78
1:B:95:LYS:H	1:B:96:SER:HA	1.46	0.78
1:D:97:PHE:HB3	1:D:98:PRO:HA	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:GLY:C	1:A:926:THR:N	2.37	0.78
1:B:433:ARG:NH2	1:B:782:ARG:O	2.16	0.78
1:D:31:GLN:HB3	1:D:32:ASN:HB3	1.65	0.78
1:A:807:VAL:O	1:A:807:VAL:HG13	1.85	0.78
1:C:811:SER:O	1:C:817:ASP:N	2.17	0.77
1:C:299:SER:OG	1:C:403:ARG:NH1	2.17	0.77
1:D:299:SER:OG	1:D:403:ARG:NH1	2.16	0.77
1:C:97:PHE:HB3	1:C:98:PRO:HA	1.66	0.77
1:A:734:GLY:O	1:A:737:VAL:HG22	1.84	0.77
1:A:97:PHE:HB3	1:A:98:PRO:HA	1.64	0.77
1:B:734:GLY:O	1:B:737:VAL:HG22	1.84	0.77
1:B:97:PHE:HB3	1:B:98:PRO:HA	1.64	0.77
1:A:31:GLN:CB	1:A:32:ASN:HB3	2.15	0.76
1:A:819:ASP:CA	1:A:820:ALA:O	2.33	0.76
1:C:31:GLN:HB3	1:C:32:ASN:HB3	1.66	0.76
1:C:986:MET:HE2	1:D:499:LEU:O	1.84	0.76
1:A:355:ILE:HD11	1:A:405:VAL:HG12	1.63	0.76
1:A:120:THR:OG1	1:A:159:PRO:HB3	1.86	0.76
1:A:717:HIS:NE2	1:A:766:GLU:OE1	2.18	0.76
1:A:246:PRO:CB	1:A:247:ALA:HB2	2.16	0.76
1:C:734:GLY:O	1:C:737:VAL:HG22	1.86	0.76
1:A:116:SER:HB3	1:A:119:ASN:OD1	1.85	0.75
1:A:194:LYS:HE3	1:A:195:PRO:HD2	1.67	0.75
1:D:734:GLY:O	1:D:737:VAL:HG22	1.85	0.75
1:D:884:GLN:O	1:D:888:LYS:HD2	1.87	0.75
1:C:184:ALA:HA	1:C:185:ALA:C	2.07	0.75
1:A:912:LEU:O	1:A:915:GLN:HG2	1.87	0.75
1:B:246:PRO:CB	1:B:247:ALA:HB2	2.16	0.75
1:B:31:GLN:CB	1:B:32:ASN:HB3	2.16	0.75
1:A:184:ALA:HA	1:A:185:ALA:CB	2.16	0.75
1:A:703:TYR:HA	1:A:706:ILE:HG22	1.66	0.75
1:A:79:MET:HG3	1:A:83:TRP:CD1	2.21	0.75
1:A:539:MET:CE	1:A:609:VAL:C	2.55	0.75
1:C:561:LYS:HG2	1:C:570:THR:OG1	1.87	0.74
1:A:79:MET:SD	1:A:106:PHE:CE2	2.80	0.74
1:A:858:GLY:HA2	1:A:941:TYR:OH	1.86	0.74
1:D:246:PRO:CB	1:D:247:ALA:HB2	2.17	0.74
1:D:31:GLN:CB	1:D:32:ASN:HB3	2.17	0.74
1:D:858:GLY:HA2	1:D:941:TYR:OH	1.87	0.74
1:C:31:GLN:CB	1:C:32:ASN:HB3	2.17	0.74
1:C:263:THR:N	1:C:264:ARG:HB2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:VAL:O	1:B:342:ILE:HG13	1.88	0.74
1:B:426:ALA:HA	1:B:645:ASN:O	1.88	0.74
1:A:355:ILE:HD12	1:A:405:VAL:HA	1.70	0.74
1:A:983:THR:HB	1:A:984:PRO:HD2	1.68	0.74
1:A:321:SER:C	1:A:323:ALA:N	2.40	0.74
1:C:433:ARG:NH2	1:C:782:ARG:O	2.21	0.74
1:B:541:MET:HG2	1:B:612:PHE:CE2	2.23	0.73
1:A:415:ASN:OD1	1:A:417:GLN:HB3	1.87	0.73
1:A:439:ARG:NH1	1:A:639:ASP:OD2	2.20	0.73
1:A:1001:LEU:HG	1:A:1002:ALA:N	2.03	0.73
1:D:619:PRO:HG2	1:D:622:ASP:HB2	1.68	0.73
1:C:1000:TYR:CZ	1:D:985:LEU:HD23	2.24	0.73
1:A:74:TRP:CD1	1:A:82:LEU:HG	2.23	0.72
1:C:246:PRO:CB	1:C:247:ALA:HB2	2.18	0.72
1:A:321:SER:O	1:A:323:ALA:N	2.21	0.72
1:A:745:LEU:O	1:A:745:LEU:CD2	2.37	0.72
1:A:184:ALA:HA	1:A:185:ALA:HB3	1.70	0.72
1:A:27:TYR:HB3	1:A:28:ALA:HA	1.71	0.72
1:A:839:LEU:HB3	1:A:840:THR:HB	1.69	0.72
1:C:858:GLY:HA2	1:C:941:TYR:OH	1.88	0.72
1:A:516:ASP:O	1:A:520:GLN:HG3	1.88	0.72
1:B:332:GLY:O	1:B:366:TRP:HA	1.89	0.71
1:B:858:GLY:HA2	1:B:941:TYR:OH	1.89	0.71
1:D:256:PRO:C	1:D:269:VAL:N	2.43	0.71
1:A:305:VAL:HG13	1:A:307:PHE:CE1	2.26	0.71
1:A:355:ILE:CD1	1:A:405:VAL:CG1	2.63	0.71
1:A:129:PHE:CZ	1:A:179:LEU:HD11	2.24	0.71
1:A:433:ARG:NH2	1:A:782:ARG:O	2.22	0.70
1:A:912:LEU:O	1:A:915:GLN:HG3	1.92	0.70
1:B:943:LYS:CB	1:B:944:THR:CB	2.70	0.70
1:C:30:LEU:HD22	1:C:190:TRP:CE3	2.26	0.70
1:A:87:THR:O	1:A:87:THR:OG1	2.04	0.70
1:A:807:VAL:CG1	1:A:807:VAL:O	2.40	0.69
1:B:23:SER:CB	1:B:24:MET:CA	2.70	0.69
1:C:95:LYS:N	1:C:96:SER:HA	2.07	0.69
1:A:806:LYS:HB3	1:A:807:VAL:HB	1.74	0.69
1:C:156:ARG:HD3	1:C:396:LEU:HD13	1.74	0.69
1:A:867:LEU:HD13	1:A:885:LEU:HD23	1.75	0.69
1:C:338:VAL:O	1:C:342:ILE:HG13	1.91	0.69
1:A:318:ASP:HB3	1:A:326:ILE:HG23	1.75	0.69
1:A:561:LYS:O	1:A:561:LYS:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:THR:HG21	1:C:342:ILE:HG12	1.75	0.69
1:A:174:ASN:OD1	1:A:175:ALA:HB3	1.92	0.69
1:A:113:ASN:O	1:A:114:PHE:HB2	1.92	0.69
1:A:413:ALA:O	1:A:635:TRP:NE1	2.26	0.69
1:A:505:ARG:HG3	1:A:505:ARG:O	1.93	0.69
1:A:989:GLY:HA2	1:B:996:PHE:CD2	2.29	0.68
1:A:338:VAL:O	1:A:342:ILE:HG13	1.92	0.68
1:A:443:ASP:HA	1:A:446:LYS:HD3	1.75	0.68
1:B:263:THR:N	1:B:264:ARG:HB2	2.09	0.68
1:A:978:MET:HB3	1:B:959:PHE:HZ	1.59	0.68
1:C:565:ASP:C	1:C:568:ASP:N	2.46	0.68
1:C:986:MET:CE	1:D:499:LEU:O	2.41	0.68
1:A:539:MET:HE2	1:A:610:ILE:N	2.08	0.68
1:A:441:MET:CE	1:A:792:VAL:HG13	2.24	0.67
1:A:469:THR:HG22	1:A:470:ASN:H	1.59	0.67
1:A:866:VAL:O	1:A:867:LEU:HG	1.94	0.67
1:C:806:LYS:CB	1:C:807:VAL:CB	2.72	0.67
1:D:338:VAL:O	1:D:342:ILE:HG13	1.93	0.67
1:D:943:LYS:CB	1:D:944:THR:CB	2.70	0.67
1:A:23:SER:HG	1:A:24:MET:HA	1.59	0.67
1:D:806:LYS:HB3	1:D:807:VAL:CB	2.25	0.67
1:A:142:MET:N	1:A:142:MET:SD	2.67	0.67
1:C:922:GLY:HA3	1:D:974:GLY:O	1.94	0.67
1:A:745:LEU:C	1:A:745:LEU:HD23	2.15	0.67
1:B:573:LEU:HG	1:B:599:PHE:CD1	2.29	0.67
1:D:170:PRO:O	1:D:180:LYS:HB3	1.95	0.67
1:A:846:LEU:H	1:A:847:ARG:HB3	1.59	0.66
1:B:95:LYS:N	1:B:96:SER:HA	2.08	0.66
1:D:251:THR:N	1:D:252:ARG:HB2	2.10	0.66
1:A:797:ILE:O	1:A:801:LEU:HG	1.95	0.66
1:C:943:LYS:CB	1:C:944:THR:CB	2.70	0.66
1:D:184:ALA:HA	1:D:185:ALA:C	2.16	0.66
1:D:95:LYS:N	1:D:96:SER:HA	2.10	0.66
1:D:343:ARG:NH1	1:D:344:ASP:OD1	2.28	0.66
1:C:985:LEU:HD23	1:D:1000:TYR:CZ	2.31	0.66
1:A:79:MET:HG3	1:A:83:TRP:NE1	2.10	0.66
1:B:812:ARG:O	1:B:823:HIS:CE1	2.49	0.66
1:C:922:GLY:CA	1:D:974:GLY:O	2.43	0.66
1:A:572:MET:HG3	1:A:573:LEU:HD13	1.77	0.66
1:C:462:ARG:HH12	1:D:990:LEU:HG	1.61	0.66
1:C:797:ILE:O	1:C:801:LEU:HG	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:PRO:O	1:D:799:ARG:HB2	1.97	0.65
1:C:979:PRO:HA	1:D:981:LEU:HD13	1.76	0.65
1:A:806:LYS:N	1:A:807:VAL:HB	2.12	0.65
1:B:304:THR:HG21	1:B:342:ILE:HG12	1.78	0.65
1:D:304:THR:HG21	1:D:342:ILE:HG12	1.78	0.65
1:D:819:ASP:CA	1:D:820:ALA:O	2.42	0.65
1:A:840:THR:HG23	1:A:840:THR:O	1.96	0.65
1:A:441:MET:HE2	1:A:792:VAL:HG13	1.78	0.65
1:B:156:ARG:HG2	1:B:275:TRP:CZ2	2.31	0.65
1:A:95:LYS:N	1:A:96:SER:HA	2.12	0.65
1:A:863:GLU:O	1:A:866:VAL:O	2.15	0.64
1:A:129:PHE:CE1	1:A:179:LEU:HD12	2.33	0.64
1:A:304:THR:HG21	1:A:342:ILE:HG12	1.80	0.64
1:A:73:SER:O	1:A:76:THR:OG1	2.14	0.64
1:A:33:ILE:CG2	1:A:140:LEU:HD11	2.27	0.64
1:A:304:THR:OG1	1:A:402:ILE:HG12	1.98	0.64
1:B:907:ALA:HA	1:B:908:LYS:HG3	1.80	0.64
1:B:184:ALA:HA	1:B:185:ALA:C	2.16	0.64
1:D:541:MET:HG2	1:D:612:PHE:CE2	2.33	0.64
1:A:126:SER:HB3	1:A:141:ASP:OD2	1.98	0.64
1:A:367:LEU:HD21	1:A:545:PHE:HE1	1.59	0.64
1:B:449:ASP:HA	1:B:452:LYS:HE3	1.79	0.64
1:C:30:LEU:HD13	1:C:190:TRP:CB	2.28	0.64
1:C:982:VAL:HG12	1:D:500:ASN:O	1.98	0.63
1:B:369:ASP:HB3	1:B:372:ASP:HB2	1.80	0.63
1:B:812:ARG:O	1:B:823:HIS:NE2	2.32	0.63
1:A:477:ARG:HD3	1:A:478:HIS:CE1	2.34	0.63
1:A:441:MET:HG2	1:A:796:THR:OG1	1.98	0.63
1:D:332:GLY:O	1:D:366:TRP:HA	1.99	0.63
1:D:982:VAL:HG11	1:D:990:LEU:HD12	1.79	0.63
1:D:433:ARG:NH2	1:D:782:ARG:O	2.32	0.63
1:C:983:THR:HG22	1:D:966:SER:HB2	1.81	0.63
1:C:541:MET:HG2	1:C:612:PHE:CE2	2.34	0.63
1:C:979:PRO:HA	1:D:981:LEU:HD22	1.81	0.63
1:D:369:ASP:HB3	1:D:372:ASP:HB2	1.80	0.63
1:C:425:ARG:CZ	1:C:425:ARG:HA	2.29	0.62
1:C:1003:ARG:NE	1:D:476:VAL:O	2.29	0.62
1:B:29:ARG:NH1	1:B:178:ILE:HG21	2.14	0.62
1:C:981:LEU:O	1:D:962:ALA:HB1	2.00	0.62
1:A:282:ASN:HA	1:A:284:TYR:CE1	2.33	0.62
1:A:321:SER:HB3	1:A:323:ALA:CA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLN:CD	1:A:808:MET:HG2	2.20	0.62
1:A:129:PHE:CZ	1:A:179:LEU:HD12	2.35	0.62
1:A:240:ARG:HG2	1:A:241:GLY:H	1.64	0.62
1:A:130:ASN:OD1	1:A:139:LEU:HD21	1.98	0.62
1:A:173:LEU:CD1	1:A:180:LYS:HG2	2.26	0.62
1:A:451:GLN:HG3	1:A:464:TRP:CZ2	2.35	0.62
1:B:157:PHE:CE2	1:B:272:MET:HG3	2.34	0.62
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.81	0.62
1:D:449:ASP:HA	1:D:452:LYS:HE3	1.81	0.62
1:D:495:LEU:HD23	1:D:510:ILE:HD13	1.82	0.62
1:B:635:TRP:CH2	1:B:637:CYS:HB2	2.35	0.62
1:A:979:PRO:HA	1:B:981:LEU:HD13	1.81	0.62
1:A:866:VAL:O	1:A:867:LEU:CB	2.45	0.61
1:B:819:ASP:CA	1:B:820:ALA:O	2.42	0.61
1:A:812:ARG:C	1:A:817:ASP:N	2.54	0.61
1:D:24:MET:N	1:D:24:MET:SD	2.73	0.61
1:A:505:ARG:O	1:A:505:ARG:CG	2.49	0.61
1:A:66:PRO:O	1:A:67:THR:OG1	2.14	0.61
1:A:559:SER:HB3	1:A:608:ASP:OD2	2.00	0.61
1:A:175:ALA:CB	1:A:179:LEU:HD13	2.30	0.61
1:A:843:SER:HG	1:A:847:ARG:HB2	1.66	0.61
1:A:133:LYS:CA	1:A:135:GLY:N	2.41	0.60
1:C:1000:TYR:CE2	1:D:985:LEU:CD2	2.83	0.60
1:A:836:PHE:O	1:A:840:THR:HG21	2.01	0.60
1:C:996:PHE:CD1	1:D:989:GLY:HA2	2.37	0.60
1:B:27:TYR:CB	1:B:28:ALA:HA	2.30	0.60
1:B:32:ASN:OD1	1:B:36:LYS:NZ	2.25	0.60
1:C:228:ALA:O	1:C:229:THR:C	2.39	0.60
1:A:174:ASN:CG	1:A:175:ALA:N	2.55	0.60
1:A:945:ASN:HB3	1:A:948:PHE:HB3	1.83	0.60
1:C:660:TYR:CE1	1:C:754:LEU:HA	2.36	0.60
1:A:439:ARG:HH22	1:A:639:ASP:CG	2.04	0.60
1:A:804:LEU:C	1:A:807:VAL:CG1	2.68	0.60
1:C:945:ASN:HB3	1:C:948:PHE:HB3	1.83	0.60
1:A:568:ASP:O	1:B:343:ARG:NH2	2.34	0.60
1:C:978:MET:O	1:D:981:LEU:HD13	2.02	0.60
1:A:841:ALA:HB3	1:A:842:GLU:HB2	1.82	0.60
1:B:361:SER:HB3	1:B:390:CYS:HB2	1.84	0.60
1:D:555:HIS:CE1	1:D:603:LEU:HB2	2.37	0.60
1:B:945:ASN:HB3	1:B:948:PHE:HB3	1.82	0.59
1:D:619:PRO:HG2	1:D:622:ASP:CB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:GLU:H	1:D:26:VAL:C	2.06	0.59
1:D:656:ASP:OD1	1:D:657:LEU:N	2.35	0.59
1:A:470:ASN:OD1	1:A:472:ARG:CB	2.50	0.59
1:A:981:LEU:HD23	1:B:962:ALA:HB1	1.84	0.59
1:B:97:PHE:HB3	1:B:98:PRO:CA	2.32	0.59
1:A:355:ILE:HD11	1:A:405:VAL:CG1	2.32	0.59
1:A:541:MET:HE3	1:A:632:ASP:HB2	1.84	0.59
1:A:657:LEU:HD12	1:A:731:THR:HG22	1.84	0.59
1:A:846:LEU:N	1:A:847:ARG:HB3	2.17	0.59
1:B:806:LYS:HB3	1:B:807:VAL:CB	2.32	0.59
1:A:739:GLN:HA	1:A:744:ILE:HD12	1.83	0.59
1:A:738:ASP:OD1	1:A:741:LYS:HE3	2.03	0.59
1:A:86:LEU:HB3	1:A:87:THR:CB	2.32	0.59
1:A:806:LYS:H	1:A:807:VAL:HB	1.67	0.59
1:B:841:ALA:HB3	1:B:842:GLU:HB2	1.85	0.59
1:B:428:ASP:OD2	1:B:431:ARG:HB2	2.03	0.58
1:C:739:GLN:HA	1:C:744:ILE:HD12	1.85	0.58
1:A:980:LEU:HD23	1:B:497:PHE:CD1	2.38	0.58
1:A:100:ARG:NH1	1:A:101:PRO:O	2.36	0.58
1:D:409:LEU:HD11	1:D:539:MET:SD	2.43	0.58
1:D:95:LYS:H	1:D:96:SER:HA	1.68	0.58
1:A:299:SER:HG	1:A:403:ARG:HH11	1.50	0.58
1:A:808:MET:CB	1:A:809:GLN:HB2	2.33	0.58
1:C:819:ASP:CA	1:C:820:ALA:O	2.45	0.58
1:C:841:ALA:HB3	1:C:842:GLU:HB2	1.84	0.58
1:D:841:ALA:HB3	1:D:842:GLU:HB2	1.84	0.58
1:A:861:GLU:OE1	1:A:945:ASN:OD1	2.22	0.58
1:A:982:VAL:O	1:A:982:VAL:HG23	2.03	0.58
1:A:922:GLY:C	1:B:974:GLY:HA3	2.24	0.58
1:A:132:SER:HA	1:A:133:LYS:HB3	1.85	0.58
1:C:361:SER:HB3	1:C:390:CYS:HB2	1.85	0.58
1:C:44:ALA:HB1	1:C:45:PRO:HA	1.85	0.58
1:C:97:PHE:HB3	1:C:98:PRO:CA	2.33	0.58
1:A:44:ALA:HB1	1:A:45:PRO:HA	1.86	0.58
1:C:449:ASP:HA	1:C:452:LYS:HE3	1.85	0.58
1:A:119:ASN:OD1	1:A:147:PHE:CE1	2.57	0.57
1:A:240:ARG:HG3	1:A:266:GLU:HG2	1.85	0.57
1:A:321:SER:C	1:A:323:ALA:CA	2.56	0.57
1:A:29:ARG:NE	1:A:133:LYS:HB2	2.18	0.57
1:A:31:GLN:HB3	1:A:32:ASN:CB	2.31	0.57
1:A:78:ASP:O	1:A:81:ALA:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HD23	1:B:510:ILE:HD13	1.87	0.57
1:B:559:SER:HA	1:B:607:LYS:HD2	1.87	0.57
1:A:177:SER:O	1:A:181:ASP:HB3	2.05	0.57
1:A:418:PHE:HZ	1:A:584:SER:HG	1.53	0.57
1:A:439:ARG:NH2	1:A:639:ASP:OD1	2.33	0.57
1:C:25:GLU:H	1:C:26:VAL:C	2.08	0.57
1:D:361:SER:HB3	1:D:390:CYS:HB2	1.86	0.57
1:C:462:ARG:NH1	1:D:990:LEU:HG	2.19	0.57
1:D:44:ALA:HB1	1:D:45:PRO:HA	1.87	0.57
1:B:44:ALA:HB1	1:B:45:PRO:HA	1.87	0.57
1:A:470:ASN:OD1	1:A:472:ARG:HB2	2.05	0.57
1:A:683:ARG:HG2	1:A:683:ARG:HH11	1.69	0.57
1:A:80:ALA:O	1:A:84:ARG:CG	2.40	0.57
1:C:416:LEU:HD12	1:C:417:GLN:N	2.20	0.57
1:A:915:GLN:N	1:A:916:PRO:HD3	2.20	0.56
1:A:928:TYR:HA	1:A:931:LEU:HD23	1.86	0.56
1:D:945:ASN:HB3	1:D:948:PHE:HB3	1.86	0.56
1:A:588:PHE:CD1	1:A:652:PRO:HG3	2.40	0.56
1:B:304:THR:HG22	1:B:305:VAL:N	2.20	0.56
1:D:576:ASP:HB3	1:D:596:ARG:HH21	1.71	0.56
1:D:83:TRP:HA	1:D:86:LEU:HD22	1.87	0.56
1:A:95:LYS:H	1:A:96:SER:HA	1.70	0.56
1:A:83:TRP:HA	1:A:86:LEU:HD22	1.86	0.56
1:C:921:ARG:O	1:C:926:THR:N	2.38	0.56
1:A:539:MET:CE	1:A:610:ILE:N	2.68	0.56
1:B:36:LYS:H	1:B:36:LYS:HD2	1.69	0.56
1:B:806:LYS:H	1:B:807:VAL:CB	2.18	0.56
1:C:860:VAL:O	1:C:863:GLU:HB2	2.06	0.56
1:A:979:PRO:CB	1:B:981:LEU:HD22	2.35	0.56
1:A:752:ASP:OD1	1:A:755:ARG:NH2	2.38	0.56
1:A:806:LYS:CA	1:A:807:VAL:HB	2.36	0.56
1:A:836:PHE:O	1:A:840:THR:CG2	2.54	0.56
1:A:886:HIS:NE2	1:A:890:CYS:SG	2.79	0.56
1:B:43:ALA:O	1:B:44:ALA:HB3	2.06	0.56
1:D:504:ASP:OD1	1:D:505:ARG:HB2	2.06	0.56
1:A:321:SER:CA	1:A:323:ALA:HA	2.35	0.56
1:A:29:ARG:CZ	1:A:133:LYS:HB2	2.36	0.55
1:A:539:MET:HE3	1:A:609:VAL:C	2.26	0.55
1:B:444:LEU:HD13	1:B:525:LEU:CD2	2.36	0.55
1:B:85:SER:HB2	1:B:86:LEU:HB2	1.88	0.55
1:C:894:PRO:HB3	1:C:929:TRP:CZ3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ASP:OD1	1:D:397:HIS:CG	2.59	0.55
1:A:267:ILE:CG2	1:A:267:ILE:O	2.54	0.55
1:A:962:ALA:HB1	1:B:981:LEU:HG	1.88	0.55
1:C:156:ARG:HD3	1:C:396:LEU:CD1	2.36	0.55
1:D:85:SER:HB2	1:D:86:LEU:HB2	1.88	0.55
1:A:886:HIS:O	1:A:889:TRP:HB3	2.07	0.55
1:C:83:TRP:HA	1:C:86:LEU:HD22	1.87	0.55
1:A:862:HIS:O	1:A:865:LYS:HB2	2.06	0.55
1:C:43:ALA:O	1:C:44:ALA:HB3	2.07	0.55
1:A:29:ARG:HD2	1:A:133:LYS:HB2	1.88	0.55
1:A:806:LYS:H	1:A:807:VAL:CB	2.19	0.55
1:B:83:TRP:HA	1:B:86:LEU:HD22	1.88	0.55
1:A:43:ALA:O	1:A:44:ALA:HB3	2.07	0.55
1:A:861:GLU:HG2	1:A:941:TYR:CZ	2.42	0.55
1:D:43:ALA:O	1:D:44:ALA:HB3	2.06	0.55
1:D:739:GLN:HA	1:D:744:ILE:HD12	1.88	0.55
1:A:459:LEU:HD11	1:B:985:LEU:HD11	1.88	0.55
1:A:603:LEU:HB3	1:A:606:LEU:HD12	1.89	0.55
1:B:953:ALA:O	1:B:955:ALA:N	2.40	0.55
1:C:85:SER:HB2	1:C:86:LEU:HB2	1.89	0.55
1:D:246:PRO:HB2	1:D:247:ALA:HB2	1.89	0.55
1:B:588:PHE:CD2	1:B:652:PRO:HG3	2.42	0.55
1:A:246:PRO:HB2	1:A:247:ALA:HB2	1.89	0.54
1:C:555:HIS:CE1	1:C:603:LEU:HB2	2.42	0.54
1:A:85:SER:HB2	1:A:86:LEU:HB2	1.87	0.54
1:A:980:LEU:N	1:B:981:LEU:HD13	2.22	0.54
1:B:739:GLN:HA	1:B:744:ILE:HD12	1.90	0.54
1:B:775:TRP:NE1	1:B:781:PRO:HD3	2.23	0.54
1:D:23:SER:CB	1:D:24:MET:CA	2.83	0.54
1:A:119:ASN:O	1:A:119:ASN:OD1	2.24	0.54
1:A:140:LEU:N	1:A:140:LEU:HD12	2.22	0.54
1:B:268:PRO:O	1:B:270:SER:N	2.40	0.54
1:C:861:GLU:O	1:C:865:LYS:N	2.31	0.54
1:B:860:VAL:O	1:B:863:GLU:HB2	2.08	0.54
1:A:979:PRO:O	1:B:959:PHE:HE1	1.86	0.54
1:A:962:ALA:HB1	1:B:981:LEU:HD23	1.89	0.54
1:C:27:TYR:CB	1:C:28:ALA:HA	2.38	0.54
1:B:25:GLU:H	1:B:26:VAL:C	2.11	0.54
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.54
1:A:736:LEU:HD22	1:A:739:GLN:OE1	2.07	0.54
1:A:953:ALA:O	1:A:955:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:CA	1:B:69:ARG:HB2	2.38	0.54
1:B:246:PRO:HB2	1:B:247:ALA:HB2	1.88	0.54
1:B:29:ARG:HH11	1:B:178:ILE:HG21	1.72	0.54
1:A:24:MET:SD	1:A:24:MET:N	2.74	0.53
1:A:361:SER:HB3	1:A:390:CYS:HB2	1.89	0.53
1:A:867:LEU:HA	1:A:881:LYS:HD2	1.89	0.53
1:D:538:TYR:CE1	1:D:635:TRP:HB2	2.43	0.53
1:A:621:ALA:HB2	1:A:629:TYR:CE2	2.44	0.53
1:C:31:GLN:HB2	1:C:32:ASN:HB3	1.91	0.53
1:C:808:MET:CB	1:C:809:GLN:HB2	2.38	0.53
1:A:541:MET:HG2	1:A:612:PHE:CE2	2.43	0.53
1:A:841:ALA:HB3	1:A:842:GLU:CB	2.38	0.53
1:B:660:TYR:N	1:B:660:TYR:CD1	2.76	0.53
1:D:794:LYS:HD3	1:D:798:ASP:OD2	2.07	0.53
1:A:321:SER:O	1:A:323:ALA:CB	2.55	0.53
1:C:332:GLY:O	1:C:366:TRP:HA	2.08	0.53
1:A:31:GLN:NE2	1:A:134:THR:OG1	2.42	0.53
1:A:367:LEU:HD22	1:A:542:VAL:CG1	2.38	0.53
1:D:495:LEU:HD23	1:D:510:ILE:CD1	2.39	0.53
1:D:363:LYS:NZ	1:D:630:ASP:OD2	2.42	0.53
1:A:29:ARG:CD	1:A:133:LYS:HB2	2.39	0.53
1:A:843:SER:O	1:A:844:ARG:HB2	2.09	0.53
1:C:978:MET:O	1:D:981:LEU:CD1	2.57	0.53
1:A:588:PHE:HD2	1:A:591:ASP:OD1	1.91	0.53
1:D:136:PRO:O	1:D:137:LEU:CB	2.57	0.53
1:D:808:MET:CB	1:D:809:GLN:HB2	2.39	0.53
1:B:419:LEU:HB2	1:B:420:PRO:HD3	1.91	0.53
1:D:321:SER:O	1:D:323:ALA:N	2.42	0.53
1:D:794:LYS:HB3	1:D:795:PRO:HD3	1.90	0.53
1:C:136:PRO:O	1:C:137:LEU:CB	2.57	0.53
1:C:841:ALA:HB3	1:C:842:GLU:CB	2.39	0.53
1:A:982:VAL:HG21	1:A:987:TYR:HD2	1.74	0.52
1:C:714:VAL:O	1:C:718:ASN:HB2	2.09	0.52
1:D:860:VAL:O	1:D:863:GLU:HB2	2.09	0.52
1:C:621:ALA:HB2	1:C:629:TYR:CE1	2.44	0.52
1:C:979:PRO:O	1:D:959:PHE:CD1	2.62	0.52
1:A:97:PHE:HB3	1:A:98:PRO:CA	2.35	0.52
1:C:603:LEU:HB3	1:C:606:LEU:HD12	1.90	0.52
1:D:841:ALA:HB3	1:D:842:GLU:CB	2.40	0.52
1:C:541:MET:HE3	1:C:632:ASP:HB2	1.91	0.52
1:A:180:LYS:HD2	1:A:183:GLY:CA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:SER:CB	1:B:822:ALA:H	2.22	0.52
1:A:270:SER:CB	1:A:684:HIS:HD2	2.22	0.52
1:A:640:PRO:O	1:A:644:GLU:HG2	2.10	0.52
1:A:806:LYS:CB	1:A:807:VAL:HB	2.39	0.52
1:C:425:ARG:NH1	1:C:647:THR:O	2.42	0.52
1:D:953:ALA:O	1:D:956:GLN:N	2.37	0.52
1:A:136:PRO:O	1:A:137:LEU:HB3	2.10	0.52
1:A:675:THR:HG21	1:A:682:ALA:HA	1.90	0.52
1:D:304:THR:HG22	1:D:305:VAL:HG12	1.91	0.52
1:D:498:LEU:O	1:D:503:PHE:HB2	2.10	0.52
1:A:136:PRO:O	1:A:137:LEU:CB	2.57	0.52
1:A:878:TYR:HB3	1:A:879:PRO:HD3	1.92	0.52
1:D:603:LEU:HB3	1:D:606:LEU:HD12	1.91	0.52
1:D:621:ALA:HB2	1:D:629:TYR:CE2	2.45	0.52
1:A:572:MET:HG3	1:A:573:LEU:CD1	2.40	0.52
1:C:136:PRO:O	1:C:137:LEU:HB3	2.10	0.52
1:A:25:GLU:H	1:A:26:VAL:C	2.13	0.51
1:A:305:VAL:HG13	1:A:307:PHE:HE1	1.70	0.51
1:A:55:ILE:HD11	1:A:83:TRP:NE1	2.24	0.51
1:B:423:GLU:O	1:B:429:LYS:HG2	2.09	0.51
1:C:308:GLU:OE1	1:C:308:GLU:HA	2.10	0.51
1:A:133:LYS:HD2	1:A:134:THR:HA	1.93	0.51
1:A:83:TRP:O	1:A:87:THR:OG1	2.26	0.51
1:A:847:ARG:NH1	1:A:851:GLU:OE2	2.43	0.51
1:D:953:ALA:O	1:D:955:ALA:N	2.42	0.51
1:A:105:ALA:HA	1:A:147:PHE:CE2	2.45	0.51
1:A:332:GLY:O	1:A:366:TRP:HA	2.10	0.51
1:A:444:LEU:HD23	1:A:796:THR:CG2	2.40	0.51
1:B:136:PRO:O	1:B:137:LEU:CB	2.58	0.51
1:B:203:TRP:HB3	1:B:236:PHE:HB3	1.93	0.51
1:B:635:TRP:CZ2	1:B:637:CYS:HB2	2.46	0.51
1:A:367:LEU:HD21	1:A:545:PHE:CD1	2.46	0.51
1:A:846:LEU:HA	1:A:849:VAL:HG23	1.93	0.51
1:B:808:MET:CB	1:B:809:GLN:HB2	2.40	0.51
1:A:980:LEU:HD22	1:B:987:TYR:CD1	2.45	0.51
1:C:986:MET:HE2	1:D:500:ASN:HA	1.92	0.51
1:A:120:THR:OG1	1:A:159:PRO:CB	2.56	0.51
1:A:864:TRP:O	1:A:867:LEU:O	2.28	0.51
1:B:498:LEU:O	1:B:503:PHE:HB2	2.10	0.51
1:A:683:ARG:NH1	1:A:683:ARG:HG2	2.26	0.51
1:B:841:ALA:HB3	1:B:842:GLU:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:VAL:HG12	1:D:199:VAL:O	2.11	0.51
1:D:97:PHE:HB3	1:D:98:PRO:CA	2.35	0.51
1:B:806:LYS:N	1:B:807:VAL:CB	2.74	0.51
1:D:136:PRO:O	1:D:137:LEU:HB3	2.10	0.51
1:A:194:LYS:HE3	1:A:195:PRO:CD	2.37	0.51
1:A:248:PRO:HG3	1:A:271:GLU:OE2	2.10	0.51
1:D:981:LEU:HD12	1:D:982:VAL:N	2.26	0.51
1:C:30:LEU:HD13	1:C:190:TRP:CG	2.46	0.50
1:D:713:ARG:HG2	1:D:768:PRO:HD3	1.93	0.50
1:A:621:ALA:HB2	1:A:629:TYR:CZ	2.46	0.50
1:A:686:ALA:O	1:A:689:ASP:HB2	2.12	0.50
1:B:287:HIS:ND1	1:B:671:LEU:HD11	2.26	0.50
1:C:246:PRO:HB2	1:C:247:ALA:HB2	1.90	0.50
1:D:279:LEU:CB	1:D:683:ARG:CZ	2.80	0.50
1:A:539:MET:CE	1:A:610:ILE:HB	2.41	0.50
1:A:824:SER:O	1:A:938:PHE:HZ	1.94	0.50
1:D:894:PRO:HB3	1:D:929:TRP:CZ3	2.47	0.50
1:A:79:MET:CG	1:A:83:TRP:NE1	2.74	0.50
1:A:957:LEU:HA	1:A:960:ILE:HD12	1.92	0.50
1:D:31:GLN:HB2	1:D:32:ASN:HB3	1.92	0.50
1:A:555:HIS:CE1	1:A:603:LEU:HB2	2.46	0.50
1:B:555:HIS:CE1	1:B:599:PHE:CD1	2.99	0.50
1:B:621:ALA:HB2	1:B:629:TYR:CE1	2.46	0.50
1:B:98:PRO:O	1:B:100:ARG:N	2.45	0.50
1:C:419:LEU:HB2	1:C:420:PRO:HD3	1.93	0.50
1:B:981:LEU:HD12	1:B:982:VAL:N	2.27	0.50
1:D:878:TYR:HB3	1:D:879:PRO:HD3	1.92	0.50
1:A:355:ILE:HD11	1:A:402:ILE:HG23	1.94	0.50
1:A:962:ALA:HB1	1:B:981:LEU:CG	2.41	0.50
1:D:419:LEU:HB2	1:D:420:PRO:HD3	1.93	0.50
1:A:985:LEU:HD13	1:A:986:MET:N	2.27	0.50
1:C:498:LEU:O	1:C:503:PHE:HB2	2.12	0.50
1:D:246:PRO:HB3	1:D:247:ALA:HB2	1.93	0.50
1:A:179:LEU:HD23	1:A:180:LYS:HB3	1.93	0.49
1:A:38:PRO:HB2	1:A:40:TRP:CE3	2.47	0.49
1:A:498:LEU:O	1:A:503:PHE:HB2	2.11	0.49
1:A:411:PRO:HD3	1:A:562:PHE:CE1	2.48	0.49
1:C:861:GLU:HG2	1:C:941:TYR:CZ	2.47	0.49
1:D:256:PRO:O	1:D:269:VAL:N	2.46	0.49
1:A:416:LEU:HD12	1:A:417:GLN:N	2.27	0.49
1:C:878:TYR:HB3	1:C:879:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:985:LEU:HD23	1:D:1000:TYR:CE2	2.47	0.49
1:D:886:HIS:O	1:D:889:TRP:HB3	2.12	0.49
1:A:953:ALA:O	1:A:956:GLN:N	2.37	0.49
1:B:931:LEU:HD12	1:B:960:ILE:HG13	1.94	0.49
1:C:30:LEU:HB3	1:C:190:TRP:CE2	2.48	0.49
1:A:439:ARG:NH2	1:A:639:ASP:CG	2.65	0.49
1:C:886:HIS:O	1:C:889:TRP:HB3	2.13	0.49
1:B:775:TRP:HE1	1:B:781:PRO:HD3	1.78	0.49
1:A:837:LYS:C	1:A:840:THR:HG22	2.33	0.49
1:C:957:LEU:HA	1:C:960:ILE:HD12	1.95	0.49
1:D:909:THR:O	1:D:912:LEU:HB2	2.12	0.49
1:D:931:LEU:HD12	1:D:960:ILE:HG13	1.95	0.49
1:A:175:ALA:HB1	1:A:179:LEU:HD13	1.93	0.49
1:A:93:ARG:N	1:A:94:GLY:HA3	2.27	0.49
1:B:136:PRO:O	1:B:137:LEU:HB3	2.13	0.49
1:B:246:PRO:HB3	1:B:247:ALA:HB2	1.92	0.49
1:B:27:TYR:CB	1:B:28:ALA:CA	2.91	0.49
1:B:878:TYR:HB3	1:B:879:PRO:HD3	1.93	0.49
1:D:843:SER:O	1:D:844:ARG:HB2	2.13	0.49
1:D:93:ARG:N	1:D:94:GLY:HA3	2.28	0.49
1:B:425:ARG:NH1	1:B:647:THR:O	2.44	0.49
1:C:98:PRO:O	1:C:100:ARG:N	2.46	0.49
1:A:825:TRP:HB2	1:A:942:TYR:CE2	2.48	0.49
1:A:866:VAL:O	1:A:867:LEU:CG	2.60	0.49
1:C:818:ASP:HB2	1:C:820:ALA:HB3	1.95	0.49
1:A:180:LYS:HD2	1:A:183:GLY:HA3	1.94	0.48
1:A:321:SER:CB	1:A:323:ALA:CA	2.91	0.48
1:A:444:LEU:HD23	1:A:796:THR:HG22	1.94	0.48
1:A:980:LEU:H	1:B:981:LEU:HD13	1.78	0.48
1:B:394:ASP:OD1	1:B:395:ALA:N	2.46	0.48
1:B:957:LEU:HA	1:B:960:ILE:HD12	1.94	0.48
1:C:68:LEU:CA	1:C:69:ARG:CB	2.90	0.48
1:D:982:VAL:HG11	1:D:990:LEU:CD1	2.43	0.48
1:A:655:PRO:HD2	1:A:731:THR:OG1	2.13	0.48
1:D:530:ASN:N	1:D:530:ASN:OD1	2.45	0.48
1:D:588:PHE:CD2	1:D:652:PRO:HG3	2.48	0.48
1:C:953:ALA:O	1:C:955:ALA:N	2.45	0.48
1:A:78:ASP:O	1:A:79:MET:C	2.51	0.48
1:B:46:LEU:HD12	1:B:201:ARG:CZ	2.42	0.48
1:A:840:THR:CG2	1:A:840:THR:O	2.60	0.48
1:B:843:SER:O	1:B:844:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:ALA:HB1	1:B:981:LEU:CD2	2.44	0.48
1:C:127:LEU:HD21	1:C:140:LEU:CG	2.44	0.48
1:C:931:LEU:HD12	1:C:960:ILE:HG13	1.95	0.48
1:C:843:SER:O	1:C:844:ARG:HB2	2.14	0.48
1:A:839:LEU:N	1:A:840:THR:HG22	2.16	0.48
1:A:79:MET:CG	1:A:83:TRP:CE2	2.96	0.48
1:B:451:GLN:HG3	1:B:464:TRP:CZ2	2.49	0.48
1:B:894:PRO:HB3	1:B:929:TRP:CZ3	2.49	0.48
1:A:34:TRP:CE3	1:A:140:LEU:HD21	2.49	0.48
1:A:410:LYS:HG2	1:A:411:PRO:N	2.29	0.48
1:A:490:ASN:OD1	1:A:490:ASN:C	2.51	0.48
1:B:149:GLU:HB3	1:B:300:LYS:HD3	1.96	0.48
1:C:413:ALA:O	1:C:635:TRP:NE1	2.47	0.48
1:D:69:ARG:CZ	1:D:74:TRP:CZ2	2.96	0.48
1:A:660:TYR:OH	1:A:758:ARG:NE	2.47	0.47
1:C:953:ALA:O	1:C:956:GLN:N	2.39	0.47
1:A:270:SER:OG	1:A:684:HIS:CD2	2.67	0.47
1:A:938:PHE:O	1:A:942:TYR:HB3	2.14	0.47
1:B:153:LEU:HB3	1:B:162:PHE:CZ	2.49	0.47
1:B:673:ARG:HA	1:B:676:GLY:C	2.34	0.47
1:D:736:LEU:HD22	1:D:739:GLN:OE1	2.14	0.47
1:A:931:LEU:HD12	1:A:960:ILE:HG13	1.96	0.47
1:B:38:PRO:HB2	1:B:40:TRP:CE3	2.49	0.47
1:B:861:GLU:HG2	1:B:941:TYR:CZ	2.49	0.47
1:C:375:ASP:N	1:C:375:ASP:OD1	2.47	0.47
1:C:94:GLY:HA2	1:C:95:LYS:HB2	1.97	0.47
1:C:479:GLY:O	1:D:1000:TYR:HE2	1.97	0.47
1:D:38:PRO:HB2	1:D:40:TRP:CE3	2.49	0.47
1:A:98:PRO:O	1:A:100:ARG:N	2.47	0.47
1:B:24:MET:N	1:B:24:MET:SD	2.74	0.47
1:C:58:HIS:CD2	1:C:98:PRO:HB3	2.50	0.47
1:D:538:TYR:HA	1:D:634:ALA:O	2.14	0.47
1:A:246:PRO:HB3	1:A:247:ALA:HB2	1.93	0.47
1:A:317:ASP:N	1:A:317:ASP:OD1	2.48	0.47
1:B:425:ARG:HD2	1:B:589:PRO:O	2.15	0.47
1:A:367:LEU:CD2	1:A:545:PHE:HE1	2.26	0.47
1:A:588:PHE:CE1	1:A:652:PRO:HG3	2.50	0.47
1:B:886:HIS:O	1:B:889:TRP:HB3	2.14	0.47
1:C:635:TRP:CH2	1:C:637:CYS:HB2	2.50	0.47
1:C:736:LEU:HD22	1:C:739:GLN:OE1	2.14	0.47
1:A:132:SER:CA	1:A:133:LYS:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD23	1:A:87:THR:CG2	2.45	0.47
1:C:820:ALA:HB1	1:C:821:ALA:CA	2.45	0.47
1:B:31:GLN:HB2	1:B:32:ASN:HB3	1.93	0.47
1:B:808:MET:H	1:B:809:GLN:HB3	1.79	0.47
1:B:996:PHE:CE1	1:B:1000:TYR:HB2	2.50	0.47
1:D:957:LEU:HA	1:D:960:ILE:HD12	1.95	0.47
1:A:199:VAL:HG12	1:A:199:VAL:O	2.15	0.47
1:A:635:TRP:CH2	1:A:637:CYS:HB2	2.50	0.47
1:A:751:TRP:CZ2	1:A:755:ARG:HD3	2.50	0.47
1:A:974:GLY:O	1:A:975:SER:CB	2.62	0.47
1:B:495:LEU:HD23	1:B:510:ILE:CD1	2.43	0.47
1:C:321:SER:OG	1:C:617:ASP:HA	2.14	0.47
1:C:38:PRO:HB2	1:C:40:TRP:CE3	2.50	0.47
1:D:246:PRO:HA	1:D:254:GLN:HB2	1.97	0.47
1:D:329:ASP:HB3	1:D:628:ASP:HB2	1.96	0.47
1:D:68:LEU:CA	1:D:69:ARG:HB2	2.45	0.47
1:A:132:SER:HA	1:A:133:LYS:CB	2.44	0.47
1:A:446:LYS:NZ	1:A:447:GLN:HB3	2.30	0.47
1:A:304:THR:HG22	1:A:305:VAL:HG12	1.97	0.46
1:D:535:ARG:NH1	1:D:564:ASP:OD2	2.48	0.46
1:D:713:ARG:HD2	1:D:765:VAL:CB	2.45	0.46
1:B:199:VAL:O	1:B:199:VAL:HG12	2.14	0.46
1:B:248:PRO:HA	1:B:249:LEU:HA	1.61	0.46
1:B:603:LEU:HB3	1:B:606:LEU:HD12	1.96	0.46
1:B:953:ALA:O	1:B:956:GLN:N	2.38	0.46
1:A:511:GLN:OE1	1:A:808:MET:HG2	2.15	0.46
1:B:491:LYS:O	1:B:494:VAL:HB	2.15	0.46
1:B:573:LEU:HG	1:B:599:PHE:CE1	2.50	0.46
1:B:663:LYS:HZ1	1:B:742:GLN:HG3	1.80	0.46
1:B:484:LEU:HG	1:B:882:VAL:HG11	1.97	0.46
1:D:203:TRP:HB3	1:D:236:PHE:HB3	1.97	0.46
1:D:559:SER:HA	1:D:607:LYS:HD2	1.97	0.46
1:B:497:PHE:HA	1:B:987:TYR:OH	2.16	0.46
1:B:555:HIS:HE1	1:B:599:PHE:CE1	2.33	0.46
1:B:713:ARG:HG2	1:B:768:PRO:HD3	1.98	0.46
1:C:153:LEU:HB3	1:C:162:PHE:CZ	2.50	0.46
1:A:515:PHE:CE1	1:A:519:LYS:HE3	2.51	0.46
1:B:363:LYS:HE3	1:B:387:LYS:HE3	1.96	0.46
1:A:837:LYS:HA	1:A:840:THR:HG21	1.96	0.46
1:B:94:GLY:HA2	1:B:95:LYS:HB2	1.98	0.46
1:C:177:SER:O	1:C:181:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:VAL:O	1:C:199:VAL:HG12	2.15	0.46
1:C:289:LYS:O	1:C:293:ARG:HG2	2.16	0.46
1:D:98:PRO:O	1:D:100:ARG:N	2.49	0.46
1:A:173:LEU:HA	1:A:174:ASN:HA	1.55	0.46
1:A:267:ILE:O	1:A:267:ILE:HG22	2.15	0.46
1:A:794:LYS:CB	1:A:795:PRO:HD3	2.46	0.46
1:A:819:ASP:N	1:A:820:ALA:O	2.49	0.46
1:B:411:PRO:CG	1:B:562:PHE:CZ	2.98	0.46
1:C:329:ASP:HB3	1:C:628:ASP:HB2	1.98	0.46
1:A:419:LEU:HB2	1:A:420:PRO:HD3	1.97	0.46
1:A:507:GLN:OE1	1:A:508:LYS:N	2.49	0.46
1:B:928:TYR:HA	1:B:931:LEU:HD23	1.98	0.46
1:C:506:ARG:HA	1:C:821:ALA:O	2.15	0.46
1:C:497:PHE:HA	1:C:987:TYR:OH	2.16	0.46
1:D:806:LYS:CB	1:D:807:VAL:CB	2.93	0.46
1:A:343:ARG:HH22	1:B:568:ASP:HB2	1.81	0.46
1:A:432:MET:C	1:A:432:MET:SD	2.95	0.46
1:A:55:ILE:HD11	1:A:83:TRP:CD1	2.51	0.46
1:B:177:SER:O	1:B:181:ASP:HB2	2.16	0.46
1:B:791:ALA:O	1:B:795:PRO:HG2	2.16	0.46
1:D:416:LEU:HD12	1:D:417:GLN:N	2.31	0.46
1:D:824:SER:O	1:D:938:PHE:HZ	1.98	0.46
1:B:329:ASP:HB3	1:B:628:ASP:HB2	1.98	0.46
1:C:985:LEU:CD2	1:D:1000:TYR:CZ	2.97	0.46
1:A:248:PRO:HA	1:A:249:LEU:HA	1.71	0.45
1:A:29:ARG:O	1:A:30:LEU:HB2	2.15	0.45
1:A:756:ARG:NH2	1:D:775:TRP:O	2.48	0.45
1:A:840:THR:H	1:A:843:SER:HA	1.80	0.45
1:C:794:LYS:HB3	1:C:795:PRO:HD3	1.99	0.45
1:C:996:PHE:C	1:C:996:PHE:CD1	2.89	0.45
1:D:938:PHE:O	1:D:942:TYR:HB3	2.16	0.45
1:A:152:ARG:HH22	1:A:360:GLY:CA	2.30	0.45
1:B:671:LEU:HD21	1:B:693:LYS:HE2	1.98	0.45
1:D:497:PHE:HA	1:D:987:TYR:OH	2.16	0.45
1:D:676:GLY:HA3	1:D:678:THR:N	2.32	0.45
1:A:245:ARG:HD2	1:A:265:THR:HG22	1.98	0.45
1:B:268:PRO:O	1:B:269:VAL:C	2.55	0.45
1:C:985:LEU:HD13	1:C:986:MET:N	2.32	0.45
1:A:451:GLN:HG3	1:A:464:TRP:CH2	2.52	0.45
1:C:139:LEU:HD22	1:C:139:LEU:HA	1.87	0.45
1:C:564:ASP:O	1:C:568:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:MET:CE	1:A:609:VAL:O	2.64	0.45
1:A:79:MET:HG3	1:A:83:TRP:CE2	2.51	0.45
1:A:866:VAL:O	1:A:867:LEU:HB2	2.15	0.45
1:B:824:SER:O	1:B:938:PHE:HZ	2.00	0.45
1:D:523:GLU:HA	1:D:526:ARG:HG2	1.99	0.45
1:D:861:GLU:HG2	1:D:941:TYR:CZ	2.52	0.45
1:A:305:VAL:CG1	1:A:307:PHE:CE1	2.98	0.45
1:C:484:LEU:HG	1:C:882:VAL:HG11	1.99	0.45
1:C:962:ALA:HB1	1:D:981:LEU:HD23	1.99	0.45
1:A:162:PHE:CE2	1:A:237:PHE:HD1	2.34	0.45
1:B:421:VAL:HG13	1:B:589:PRO:HA	1.99	0.45
1:B:69:ARG:HG3	1:B:70:TYR:N	2.31	0.45
1:B:946:PRO:O	1:B:950:TRP:HD1	2.00	0.45
1:D:946:PRO:O	1:D:950:TRP:HD1	1.99	0.45
1:A:133:LYS:N	1:A:135:GLY:HA3	2.32	0.45
1:A:94:GLY:HA2	1:A:95:LYS:CB	2.47	0.45
1:A:953:ALA:O	1:A:954:GLY:C	2.55	0.45
1:C:248:PRO:HA	1:C:249:LEU:HA	1.72	0.45
1:C:24:MET:SD	1:C:24:MET:N	2.75	0.45
1:A:289:LYS:O	1:A:293:ARG:HG2	2.17	0.45
1:A:372:ASP:OD1	1:A:374:GLY:N	2.39	0.45
1:A:523:GLU:HA	1:A:526:ARG:HG2	1.99	0.45
1:A:427:LYS:N	1:A:645:ASN:O	2.47	0.45
1:B:673:ARG:C	1:B:676:GLY:H	2.21	0.45
1:D:714:VAL:O	1:D:718:ASN:HB2	2.17	0.45
1:D:985:LEU:HD13	1:D:986:MET:N	2.32	0.45
1:A:48:LEU:C	1:A:48:LEU:HD12	2.38	0.44
1:A:565:ASP:OD2	1:A:568:ASP:N	2.50	0.44
1:A:717:HIS:HE2	1:A:766:GLU:CD	2.19	0.44
1:A:980:LEU:N	1:A:980:LEU:HD12	2.32	0.44
1:C:938:PHE:O	1:C:942:TYR:HB3	2.17	0.44
1:A:272:MET:O	1:A:275:TRP:HB3	2.18	0.44
1:B:806:LYS:CB	1:B:807:VAL:CB	2.95	0.44
1:D:818:ASP:HB2	1:D:820:ALA:HB3	1.99	0.44
1:A:184:ALA:HA	1:A:185:ALA:HB2	1.98	0.44
1:A:29:ARG:O	1:A:30:LEU:CB	2.65	0.44
1:A:996:PHE:C	1:A:996:PHE:CD1	2.90	0.44
1:C:30:LEU:HD22	1:C:190:TRP:CD2	2.51	0.44
1:D:248:PRO:HA	1:D:249:LEU:HA	1.71	0.44
1:D:928:TYR:HA	1:D:931:LEU:HD23	1.99	0.44
1:A:189:ARG:HB2	1:A:189:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:TRP:CZ2	1:B:755:ARG:HD3	2.52	0.44
1:C:523:GLU:HA	1:C:526:ARG:HG2	1.98	0.44
1:C:806:LYS:CA	1:C:807:VAL:CB	2.95	0.44
1:C:996:PHE:CE1	1:D:989:GLY:HA2	2.51	0.44
1:A:140:LEU:HD23	1:A:142:MET:CE	2.47	0.44
1:A:979:PRO:HD2	1:B:959:PHE:CZ	2.52	0.44
1:B:977:GLY:O	1:B:979:PRO:HD3	2.17	0.44
1:A:355:ILE:HD11	1:A:402:ILE:CG2	2.47	0.44
1:A:325:LYS:HE3	1:A:622:ASP:OD2	2.17	0.44
1:B:894:PRO:HB2	1:B:910:ALA:HA	2.00	0.44
1:B:94:GLY:HA2	1:B:95:LYS:CB	2.48	0.44
1:C:491:LYS:O	1:C:494:VAL:HB	2.17	0.44
1:C:824:SER:O	1:C:938:PHE:HZ	2.01	0.44
1:A:470:ASN:OD1	1:A:472:ARG:NH1	2.51	0.44
1:A:477:ARG:CD	1:A:478:HIS:CE1	2.99	0.44
1:A:713:ARG:HG2	1:A:768:PRO:HD3	2.00	0.44
1:A:808:MET:H	1:A:809:GLN:HB3	1.83	0.44
1:B:289:LYS:O	1:B:293:ARG:HG2	2.18	0.44
1:B:953:ALA:O	1:B:954:GLY:C	2.55	0.44
1:A:189:ARG:HB2	1:A:189:ARG:HH11	1.83	0.44
1:A:660:TYR:CE2	1:A:754:LEU:HA	2.52	0.44
1:A:791:ALA:O	1:A:795:PRO:HG2	2.18	0.44
1:B:28:ALA:HB3	1:B:134:THR:HG22	2.00	0.44
1:C:246:PRO:HB3	1:C:247:ALA:HB2	1.95	0.44
1:D:618:ILE:CG1	1:D:623:LYS:HG3	2.47	0.44
1:A:194:LYS:CE	1:A:195:PRO:HD2	2.41	0.44
1:A:660:TYR:N	1:A:660:TYR:CD1	2.86	0.44
1:A:441:MET:HE3	1:A:792:VAL:CG1	2.48	0.44
1:A:441:MET:HE3	1:A:792:VAL:HG13	1.99	0.44
1:B:755:ARG:HA	1:B:759:LEU:HB2	1.99	0.44
1:C:263:THR:CB	1:C:264:ARG:HE	2.31	0.44
1:C:29:ARG:O	1:C:30:LEU:HB2	2.17	0.44
1:C:840:THR:HA	1:C:843:SER:CB	2.48	0.44
1:A:270:SER:HA	1:A:687:VAL:HG11	1.99	0.43
1:B:938:PHE:O	1:B:942:TYR:HB3	2.18	0.43
1:C:304:THR:HG22	1:C:305:VAL:N	2.32	0.43
1:A:714:VAL:O	1:A:718:ASN:HB2	2.18	0.43
1:A:949:VAL:CG2	1:A:950:TRP:N	2.80	0.43
1:A:753:ARG:CZ	1:D:774:VAL:HG11	2.49	0.43
1:A:79:MET:O	1:A:83:TRP:N	2.36	0.43
1:B:211:ALA:HB2	1:B:231:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:MET:HE3	1:D:632:ASP:HB2	2.00	0.43
1:D:791:ALA:O	1:D:795:PRO:HG2	2.18	0.43
1:A:395:ALA:HA	1:A:398:ARG:NH1	2.33	0.43
1:C:263:THR:CA	1:C:264:ARG:HB2	2.48	0.43
1:C:27:TYR:N	1:C:186:GLN:HG2	2.33	0.43
1:C:270:SER:HA	1:C:687:VAL:HG11	2.01	0.43
1:D:484:LEU:HG	1:D:882:VAL:HG11	2.00	0.43
1:A:794:LYS:HB3	1:A:795:PRO:HD3	2.00	0.43
1:B:535:ARG:HB2	1:B:639:ASP:HB2	2.00	0.43
1:B:287:HIS:HB2	1:B:690:MET:HG3	2.00	0.43
1:B:820:ALA:HB1	1:B:821:ALA:CA	2.47	0.43
1:B:506:ARG:HA	1:B:821:ALA:O	2.18	0.43
1:A:184:ALA:CA	1:A:185:ALA:CB	2.90	0.43
1:A:245:ARG:HA	1:A:246:PRO:HD3	1.90	0.43
1:A:568:ASP:OD1	1:A:569:THR:N	2.52	0.43
1:A:760:GLY:HA3	1:A:761:GLY:HA3	1.66	0.43
1:B:133:LYS:HA	1:B:134:THR:HA	1.80	0.43
1:B:263:THR:CA	1:B:264:ARG:HB2	2.49	0.43
1:A:986:MET:CE	1:B:462:ARG:HD3	2.48	0.43
1:A:274:ASP:HA	1:A:279:LEU:HG	2.00	0.43
1:B:270:SER:HA	1:B:687:VAL:HG11	2.01	0.43
1:D:133:LYS:HA	1:D:134:THR:HA	1.78	0.43
1:A:140:LEU:N	1:A:140:LEU:CD1	2.81	0.43
1:A:321:SER:OG	1:A:617:ASP:HA	2.18	0.43
1:C:808:MET:HB3	1:C:809:GLN:HB2	2.01	0.43
1:D:395:ALA:HA	1:D:398:ARG:NH1	2.34	0.43
1:D:840:THR:HA	1:D:843:SER:CB	2.49	0.43
1:A:34:TRP:HB3	1:A:198:LEU:HD13	2.01	0.43
1:A:463:GLN:HE21	1:A:997:VAL:HG21	1.83	0.43
1:B:113:ASN:O	1:B:114:PHE:HB2	2.19	0.43
1:B:87:THR:HA	1:B:88:GLN:C	2.38	0.43
1:C:29:ARG:O	1:C:30:LEU:CB	2.67	0.43
1:C:840:THR:H	1:C:843:SER:HA	1.84	0.43
1:D:245:ARG:HA	1:D:246:PRO:HD3	1.79	0.43
1:D:251:THR:CA	1:D:252:ARG:HB2	2.48	0.43
1:D:287:HIS:CD2	1:D:288:LEU:HD23	2.54	0.43
1:D:635:TRP:CH2	1:D:637:CYS:HB2	2.53	0.43
1:D:270:SER:HA	1:D:687:VAL:HG11	2.01	0.43
1:D:463:GLN:HE21	1:D:997:VAL:HG21	1.84	0.43
1:A:886:HIS:CD2	1:A:890:CYS:SG	3.11	0.42
1:A:94:GLY:HA2	1:A:95:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:VAL:HG13	1:C:589:PRO:HA	2.01	0.42
1:D:953:ALA:O	1:D:954:GLY:C	2.57	0.42
1:C:979:PRO:CA	1:D:981:LEU:HD22	2.48	0.42
1:B:29:ARG:O	1:B:30:LEU:HB2	2.20	0.42
1:C:423:GLU:O	1:C:429:LYS:HG2	2.19	0.42
1:C:554:VAL:HG21	1:C:610:ILE:HD11	2.02	0.42
1:C:676:GLY:HA3	1:C:678:THR:N	2.34	0.42
1:D:413:ALA:O	1:D:635:TRP:NE1	2.52	0.42
1:A:490:ASN:OD1	1:A:492:GLY:N	2.52	0.42
1:A:491:LYS:O	1:A:494:VAL:HB	2.19	0.42
1:A:69:ARG:CG	1:A:70:TYR:N	2.81	0.42
1:A:974:GLY:O	1:A:975:SER:OG	2.24	0.42
1:B:825:TRP:HB2	1:B:942:TYR:CE2	2.55	0.42
1:B:913:LEU:HD13	1:B:929:TRP:HE3	1.84	0.42
1:C:94:GLY:HA2	1:C:95:LYS:CB	2.48	0.42
1:A:321:SER:O	1:A:322:PRO:C	2.45	0.42
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.85	0.42
1:A:561:LYS:HD3	1:A:563:ARG:NH1	2.34	0.42
1:A:85:SER:N	1:A:86:LEU:HB2	2.35	0.42
1:C:752:ASP:HA	1:C:755:ARG:NH2	2.34	0.42
1:C:760:GLY:HA3	1:C:761:GLY:HA3	1.70	0.42
1:D:211:ALA:HB2	1:D:231:LYS:O	2.20	0.42
1:A:410:LYS:HG2	1:A:411:PRO:O	2.20	0.42
1:A:554:VAL:HG21	1:A:610:ILE:HD11	2.00	0.42
1:A:660:TYR:HE2	1:A:754:LEU:HA	1.85	0.42
1:A:808:MET:HB3	1:A:809:GLN:HB2	1.99	0.42
1:B:760:GLY:HA3	1:B:761:GLY:HA3	1.75	0.42
1:C:621:ALA:HB2	1:C:629:TYR:CZ	2.55	0.42
1:C:812:ARG:C	1:C:817:ASP:N	2.72	0.42
1:A:442:ASN:O	1:A:446:LYS:HB3	2.20	0.42
1:A:808:MET:N	1:A:809:GLN:HB3	2.34	0.42
1:A:837:LYS:C	1:A:840:THR:CG2	2.88	0.42
1:A:886:HIS:O	1:A:890:CYS:N	2.42	0.42
1:A:928:TYR:OH	1:B:963:GLN:NE2	2.52	0.42
1:C:287:HIS:CD2	1:C:288:LEU:HD23	2.55	0.42
1:D:538:TYR:CZ	1:D:635:TRP:HB2	2.54	0.42
1:A:455:VAL:CG2	1:A:461:PHE:CE1	3.02	0.42
1:A:470:ASN:OD1	1:A:472:ARG:HB3	2.20	0.42
1:A:510:ILE:HD13	1:A:510:ILE:HG21	1.52	0.42
1:A:843:SER:OG	1:A:847:ARG:CB	2.57	0.42
1:B:155:ARG:NH2	1:B:401:GLU:OE2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:HIS:CE1	1:B:599:PHE:CE1	3.07	0.42
1:D:564:ASP:HB3	1:D:571:TYR:HE2	1.85	0.42
1:A:175:ALA:HB3	1:A:179:LEU:HD22	2.02	0.42
1:A:448:PHE:CE1	1:A:518:GLN:HG2	2.55	0.42
1:B:523:GLU:HA	1:B:526:ARG:HG2	2.02	0.42
1:C:25:GLU:CB	1:C:26:VAL:HG22	2.50	0.42
1:C:85:SER:N	1:C:86:LEU:HB2	2.35	0.42
1:D:155:ARG:NH2	1:D:401:GLU:OE2	2.53	0.42
1:A:25:GLU:CB	1:A:26:VAL:HG22	2.50	0.42
1:A:152:ARG:HH22	1:A:360:GLY:N	2.18	0.42
1:A:355:ILE:HD12	1:A:404:SER:O	2.19	0.42
1:A:539:MET:HE2	1:A:610:ILE:HB	2.01	0.42
1:A:620:LEU:O	1:A:621:ALA:C	2.57	0.42
1:C:155:ARG:NH2	1:C:401:GLU:OE2	2.53	0.42
1:D:29:ARG:O	1:D:30:LEU:CB	2.68	0.42
1:D:29:ARG:O	1:D:30:LEU:HB2	2.19	0.42
1:D:760:GLY:HA3	1:D:761:GLY:HA3	1.74	0.42
1:D:825:TRP:HB2	1:D:942:TYR:CE2	2.55	0.42
1:D:94:GLY:HA2	1:D:95:LYS:CB	2.50	0.42
1:B:25:GLU:CB	1:B:26:VAL:HG22	2.50	0.42
1:B:287:HIS:CD2	1:B:288:LEU:HD23	2.55	0.42
1:B:794:LYS:HB3	1:B:795:PRO:HD3	2.01	0.42
1:C:138:PHE:HE1	1:C:168:PRO:HG2	1.85	0.42
1:C:791:ALA:O	1:C:795:PRO:HG2	2.19	0.42
1:C:943:LYS:CA	1:C:944:THR:CB	2.98	0.42
1:D:943:LYS:CA	1:D:944:THR:CB	2.97	0.42
1:A:287:HIS:CD2	1:A:288:LEU:HD23	2.54	0.41
1:A:86:LEU:N	1:A:87:THR:C	2.74	0.41
1:A:946:PRO:O	1:A:950:TRP:HD1	2.02	0.41
1:D:23:SER:CB	1:D:26:VAL:O	2.68	0.41
1:D:808:MET:H	1:D:809:GLN:HB3	1.84	0.41
1:D:94:GLY:HA2	1:D:95:LYS:HB2	2.01	0.41
1:A:179:LEU:HD23	1:A:180:LYS:CB	2.50	0.41
1:A:284:TYR:CE2	1:A:285:GLN:HG2	2.54	0.41
1:A:306:THR:HA	1:A:399:THR:HA	2.02	0.41
1:A:524:VAL:HG12	1:A:530:ASN:HD21	1.85	0.41
1:B:151:CYS:SG	1:B:154:THR:HG23	2.60	0.41
1:B:187:VAL:O	1:B:190:TRP:HB3	2.20	0.41
1:B:86:LEU:N	1:B:87:THR:C	2.74	0.41
1:C:808:MET:H	1:C:809:GLN:HB3	1.86	0.41
1:D:579:VAL:HG12	1:D:638:TRP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HB3	1:A:162:PHE:CZ	2.55	0.41
1:A:484:LEU:HG	1:A:882:VAL:HG11	2.02	0.41
1:A:978:MET:O	1:A:980:LEU:HD12	2.20	0.41
1:B:840:THR:HA	1:B:843:SER:CB	2.50	0.41
1:B:943:LYS:CA	1:B:944:THR:CB	2.98	0.41
1:D:635:TRP:CZ2	1:D:637:CYS:HB2	2.56	0.41
1:A:161:ARG:NH2	1:A:267:ILE:HG22	2.34	0.41
1:A:173:LEU:N	1:A:173:LEU:HD12	2.35	0.41
1:A:941:TYR:HD1	1:A:944:THR:HG21	1.85	0.41
1:B:487:LEU:HD21	1:B:954:GLY:HA3	2.02	0.41
1:B:982:VAL:O	1:B:983:THR:C	2.58	0.41
1:D:455:VAL:O	1:D:505:ARG:CG	2.68	0.41
1:D:660:TYR:N	1:D:660:TYR:CD1	2.88	0.41
1:D:806:LYS:H	1:D:807:VAL:CB	2.33	0.41
1:B:355:ILE:CG1	1:B:405:VAL:HG12	2.50	0.41
1:A:572:MET:CE	1:B:572:MET:CG	2.98	0.41
1:D:794:LYS:CB	1:D:795:PRO:HD3	2.50	0.41
1:A:804:LEU:O	1:A:807:VAL:CG1	2.69	0.41
1:A:863:GLU:HG3	1:A:888:LYS:NZ	2.35	0.41
1:B:304:THR:HG22	1:B:305:VAL:HG12	2.03	0.41
1:B:365:MET:HG2	1:B:629:TYR:O	2.20	0.41
1:D:151:CYS:SG	1:D:154:THR:HG23	2.60	0.41
1:D:246:PRO:HB2	1:D:247:ALA:CB	2.51	0.41
1:D:274:ASP:HA	1:D:279:LEU:HG	2.03	0.41
1:D:790:PHE:O	1:D:795:PRO:HD3	2.20	0.41
1:B:268:PRO:HB2	1:B:270:SER:OG	2.20	0.41
1:B:349:SER:O	1:B:350:ASP:HB2	2.21	0.41
1:C:640:PRO:O	1:C:644:GLU:HG2	2.20	0.41
1:C:688:TYR:O	1:C:692:ASN:HB2	2.21	0.41
1:D:153:LEU:HB3	1:D:162:PHE:CZ	2.55	0.41
1:A:455:VAL:HG22	1:A:461:PHE:CE1	2.56	0.41
1:A:766:GLU:H	1:A:766:GLU:CD	2.23	0.41
1:B:29:ARG:O	1:B:30:LEU:CB	2.69	0.41
1:B:806:LYS:CA	1:B:807:VAL:CB	2.98	0.41
1:C:25:GLU:N	1:C:26:VAL:C	2.74	0.41
1:D:660:TYR:CE2	1:D:754:LEU:HA	2.55	0.41
1:D:85:SER:N	1:D:86:LEU:HB2	2.36	0.41
1:A:1000:TYR:O	1:A:1000:TYR:CD1	2.73	0.41
1:B:173:LEU:HA	1:B:174:ASN:HA	1.82	0.41
1:A:986:MET:HE2	1:B:499:LEU:O	2.20	0.41
1:A:343:ARG:NH2	1:B:568:ASP:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:O	1:B:731:THR:CB	2.68	0.41
1:D:129:PHE:CZ	1:D:168:PRO:HB2	2.56	0.41
1:A:329:ASP:HB3	1:A:628:ASP:HB2	2.03	0.41
1:A:943:LYS:CB	1:A:944:THR:CB	2.89	0.41
1:B:31:GLN:CB	1:B:32:ASN:CB	2.95	0.41
1:B:333:ARG:NE	1:B:380:GLU:OE2	2.40	0.41
1:C:113:ASN:O	1:C:114:PHE:HB2	2.21	0.41
1:D:491:LYS:O	1:D:494:VAL:HB	2.20	0.41
1:D:575:THR:OG1	1:D:576:ASP:N	2.54	0.41
1:D:808:MET:HB3	1:D:809:GLN:HB2	2.03	0.41
1:C:981:LEU:HB2	1:D:962:ALA:HB1	2.02	0.41
1:C:245:ARG:HD2	1:C:245:ARG:O	2.21	0.41
1:C:69:ARG:HG3	1:C:70:TYR:N	2.35	0.41
1:C:463:GLN:HE21	1:C:997:VAL:HG21	1.86	0.41
1:D:187:VAL:O	1:D:190:TRP:HB3	2.20	0.41
1:D:554:VAL:HG21	1:D:610:ILE:HD11	2.03	0.41
1:A:367:LEU:HG	1:A:367:LEU:H	1.84	0.40
1:A:521:ARG:HB3	1:A:521:ARG:HE	1.61	0.40
1:A:532:HIS:CG	1:A:533:VAL:N	2.88	0.40
1:A:555:HIS:C	1:A:555:HIS:CD2	2.94	0.40
1:C:68:LEU:CA	1:C:69:ARG:HB2	2.51	0.40
1:D:27:TYR:CB	1:D:28:ALA:HA	2.51	0.40
1:D:446:LYS:NZ	1:D:447:GLN:HB3	2.37	0.40
1:A:119:ASN:OD1	1:A:147:PHE:HE1	2.03	0.40
1:A:122:VAL:HG21	1:A:148:ASP:OD2	2.20	0.40
1:A:368:MET:HE2	1:A:368:MET:HB2	1.87	0.40
1:B:554:VAL:HG21	1:B:610:ILE:HD11	2.03	0.40
1:B:818:ASP:HB2	1:B:820:ALA:HB3	2.03	0.40
1:C:481:VAL:HG13	1:C:493:GLU:HG2	2.03	0.40
1:A:675:THR:CG2	1:A:682:ALA:HA	2.51	0.40
1:A:986:MET:HE2	1:B:500:ASN:HA	2.04	0.40
1:B:25:GLU:HB2	1:B:26:VAL:CG2	2.52	0.40
1:B:428:ASP:CG	1:B:431:ARG:HB2	2.41	0.40
1:C:395:ALA:HA	1:C:398:ARG:NH1	2.37	0.40
1:C:825:TRP:HB2	1:C:942:TYR:CE2	2.57	0.40
1:D:751:TRP:CZ2	1:D:755:ARG:HD3	2.56	0.40
1:A:23:SER:HB2	1:A:25:GLU:OE1	2.21	0.40
1:A:405:VAL:HG23	1:A:407:THR:CG2	2.52	0.40
1:A:657:LEU:CD1	1:A:731:THR:HG22	2.50	0.40
1:B:154:THR:HA	1:B:162:PHE:CE1	2.57	0.40
1:B:507:GLN:OE1	1:B:508:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:GLU:N	1:D:683:ARG:CZ	2.85	0.40
1:A:247:ALA:HB1	1:A:248:PRO:HD2	2.04	0.40
1:A:894:PRO:HD3	1:A:929:TRP:CE2	2.57	0.40
1:B:689:ASP:O	1:B:692:ASN:HB3	2.20	0.40
1:B:703:TYR:HE2	1:B:747:ASP:HA	1.87	0.40
1:B:86:LEU:HB3	1:B:87:THR:CB	2.51	0.40
1:C:794:LYS:CB	1:C:795:PRO:HD3	2.51	0.40
1:C:953:ALA:O	1:C:954:GLY:C	2.60	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	904/1034 (87%)	779 (86%)	90 (10%)	35 (4%)	4	28
1	B	888/1034 (86%)	779 (88%)	84 (10%)	25 (3%)	6	37
1	C	888/1034 (86%)	786 (88%)	75 (8%)	27 (3%)	5	35
1	D	886/1034 (86%)	787 (89%)	71 (8%)	28 (3%)	5	33
All	All	3566/4136 (86%)	3131 (88%)	320 (9%)	115 (3%)	5	33

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	88	GLN
1	A	133	LYS
1	A	137	LEU
1	A	184	ALA
1	A	243	ASP
1	A	413	ALA

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Mol	Chain	Res	Type
1	A	807	VAL
1	A	820	ALA
1	A	867	LEU
1	A	944	THR
1	A	954	GLY
1	B	88	GLN
1	B	137	LEU
1	B	243	ASP
1	B	248	PRO
1	B	413	ALA
1	B	820	ALA
1	B	944	THR
1	B	954	GLY
1	C	88	GLN
1	C	137	LEU
1	C	243	ASP
1	C	413	ALA
1	C	807	VAL
1	C	820	ALA
1	C	944	THR
1	C	954	GLY
1	D	88	GLN
1	D	117	ARG
1	D	137	LEU
1	D	243	ASP
1	D	576	ASP
1	D	807	VAL
1	D	820	ALA
1	D	944	THR
1	D	954	GLY
1	A	30	LEU
1	A	31	GLN
1	A	95	LYS
1	A	97	PHE
1	A	99	GLU
1	A	117	ARG
1	A	131	PRO
1	A	185	ALA
1	A	844	ARG
1	B	95	LYS
1	B	99	GLU
1	B	117	ARG

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Mol	Chain	Res	Type
1	B	211	ALA
1	B	807	VAL
1	C	30	LEU
1	C	69	ARG
1	C	95	LYS
1	C	99	GLU
1	C	117	ARG
1	D	95	LYS
1	D	97	PHE
1	D	99	GLU
1	D	211	ALA
1	D	329	ASP
1	D	413	ALA
1	A	86	LEU
1	A	114	PHE
1	A	134	THR
1	A	561	LYS
1	A	764	SER
1	B	30	LEU
1	B	86	LEU
1	B	97	PHE
1	B	269	VAL
1	B	561	LYS
1	B	844	ARG
1	C	31	GLN
1	C	86	LEU
1	C	97	PHE
1	C	248	PRO
1	C	264	ARG
1	C	329	ASP
1	C	561	LYS
1	C	844	ARG
1	D	30	LEU
1	D	31	GLN
1	D	86	LEU
1	D	844	ARG
1	A	89	LEU
1	B	89	LEU
1	B	764	SER
1	C	89	LEU
1	D	69	ARG
1	D	89	LEU

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Mol	Chain	Res	Type
1	D	561	LYS
1	A	481	VAL
1	A	847	ARG
1	B	31	GLN
1	B	264	ARG
1	C	809	GLN
1	C	847	ARG
1	D	322	PRO
1	A	248	PRO
1	A	809	GLN
1	B	908	LYS
1	C	100	ARG
1	D	100	ARG
1	D	809	GLN
1	A	100	ARG
1	A	267	ILE
1	B	100	ARG
1	A	175	ALA
1	A	136	PRO
1	C	26	VAL
1	C	136	PRO
1	D	66	PRO
1	D	26	VAL
1	D	136	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	775/856 (90%)	695 (90%)	80 (10%)	9	36
1	B	655/856 (76%)	585 (89%)	70 (11%)	8	34
1	C	655/856 (76%)	577 (88%)	78 (12%)	6	28
1	D	655/856 (76%)	578 (88%)	77 (12%)	6	29
All	All	2740/3424 (80%)	2435 (89%)	305 (11%)	8	32

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	SER
1	A	24	MET
1	A	36	LYS
1	A	39	ARG
1	A	40	TRP
1	A	48	LEU
1	A	67	THR
1	A	69	ARG
1	A	71	ASP
1	A	78	ASP
1	A	90	ASP
1	A	126	SER
1	A	133	LYS
1	A	134	THR
1	A	141	ASP
1	A	142	MET
1	A	145	LEU
1	A	146	ARG
1	A	153	LEU
1	A	178	ILE
1	A	195	PRO
1	A	197	SER
1	A	227	LYS
1	A	229	THR
1	A	245	ARG
1	A	249	LEU
1	A	267	ILE
1	A	317	ASP
1	A	341	LYS
1	A	349	SER
1	A	392	ASP
1	A	394	ASP
1	A	415	ASN
1	A	416	LEU
1	A	432	MET
1	A	446	LYS
1	A	452	LYS
1	A	457	ARG
1	A	459	LEU
1	A	468	CYS
1	A	469	THR

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Mol	Chain	Res	Type
1	A	483	PHE
1	A	495	LEU
1	A	521	ARG
1	A	530	ASN
1	A	544	ASP
1	A	560	SER
1	A	570	THR
1	A	573	LEU
1	A	577	CYS
1	A	620	LEU
1	A	647	THR
1	A	678	THR
1	A	717	HIS
1	A	728	LEU
1	A	740	SER
1	A	742	GLN
1	A	745	LEU
1	A	756	ARG
1	A	767	ASP
1	A	780	GLU
1	A	804	LEU
1	A	807	VAL
1	A	808	MET
1	A	817	ASP
1	A	840	THR
1	A	861	GLU
1	A	862	HIS
1	A	866	VAL
1	A	868	MET
1	A	877	THR
1	A	926	THR
1	A	927	SER
1	A	949	VAL
1	A	951	GLN
1	A	959	PHE
1	A	985	LEU
1	A	1001	LEU
1	A	1003	ARG
1	B	36	LYS
1	B	40	TRP
1	B	66	PRO
1	B	67	THR

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Mol	Chain	Res	Type
1	B	117	ARG
1	B	126	SER
1	B	145	LEU
1	B	153	LEU
1	B	195	PRO
1	B	197	SER
1	B	227	LYS
1	B	230	PHE
1	B	245	ARG
1	B	248	PRO
1	B	249	LEU
1	B	267	LEU
1	B	316	THR
1	B	319	ILE
1	B	336	ARG
1	B	337	SER
1	B	341	LYS
1	B	363	LYS
1	B	375	ASP
1	B	392	ASP
1	B	394	ASP
1	B	411	PRO
1	B	416	LEU
1	B	427	LYS
1	B	431	ARG
1	B	452	LYS
1	B	455	VAL
1	B	468	CYS
1	B	469	THR
1	B	483	PHE
1	B	495	LEU
1	B	510	ILE
1	B	527	THR
1	B	530	ASN
1	B	544	ASP
1	B	564	ASP
1	B	569	THR
1	B	570	THR
1	B	573	LEU
1	B	613	PRO
1	B	620	LEU
1	B	647	THR

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Mol	Chain	Res	Type
1	B	678	THR
1	B	683	ARG
1	B	689	ASP
1	B	740	SER
1	B	741	LYS
1	B	742	GLN
1	B	765	VAL
1	B	767	ASP
1	B	774	VAL
1	B	775	TRP
1	B	804	LEU
1	B	808	MET
1	B	817	ASP
1	B	840	THR
1	B	844	ARG
1	B	861	GLU
1	B	877	THR
1	B	916	PRO
1	B	926	THR
1	B	949	VAL
1	B	951	GLN
1	B	985	LEU
1	B	998	LYS
1	B	1003	ARG
1	C	36	LYS
1	C	40	TRP
1	C	66	PRO
1	C	67	THR
1	C	84	ARG
1	C	90	ASP
1	C	126	SER
1	C	139	LEU
1	C	145	LEU
1	C	153	LEU
1	C	181	ASP
1	C	195	PRO
1	C	197	SER
1	C	227	LYS
1	C	230	PHE
1	C	245	ARG
1	C	248	PRO
1	C	249	LEU

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Mol	Chain	Res	Type
1	C	267	LEU
1	C	268	PRO
1	C	316	THR
1	C	319	ILE
1	C	336	ARG
1	C	341	LYS
1	C	375	ASP
1	C	392	ASP
1	C	411	PRO
1	C	416	LEU
1	C	427	LYS
1	C	451	GLN
1	C	452	LYS
1	C	455	VAL
1	C	468	CYS
1	C	469	THR
1	C	483	PHE
1	C	495	LEU
1	C	499	LEU
1	C	510	ILE
1	C	521	ARG
1	C	527	THR
1	C	530	ASN
1	C	532	HIS
1	C	544	ASP
1	C	560	SER
1	C	564	ASP
1	C	565	ASP
1	C	571	TYR
1	C	573	LEU
1	C	577	CYS
1	C	613	PRO
1	C	620	LEU
1	C	641	ASP
1	C	647	THR
1	C	650	ASP
1	C	672	VAL
1	C	678	THR
1	C	710	TYR
1	C	728	LEU
1	C	740	SER
1	C	742	GLN

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Mol	Chain	Res	Type
1	C	773	ASP
1	C	775	TRP
1	C	802	GLU
1	C	804	LEU
1	C	808	MET
1	C	817	ASP
1	C	840	THR
1	C	849	VAL
1	C	861	GLU
1	C	877	THR
1	C	916	PRO
1	C	926	THR
1	C	949	VAL
1	C	951	GLN
1	C	981	LEU
1	C	982	VAL
1	C	985	LEU
1	C	1003	ARG
1	D	36	LYS
1	D	40	TRP
1	D	66	PRO
1	D	67	THR
1	D	71	ASP
1	D	90	ASP
1	D	99	GLU
1	D	117	ARG
1	D	126	SER
1	D	145	LEU
1	D	153	LEU
1	D	195	PRO
1	D	230	PHE
1	D	248	PRO
1	D	249	LEU
1	D	255	LEU
1	D	256	PRO
1	D	319	ILE
1	D	341	LYS
1	D	375	ASP
1	D	392	ASP
1	D	411	PRO
1	D	416	LEU
1	D	427	LYS

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Mol	Chain	Res	Type
1	D	446	LYS
1	D	452	LYS
1	D	455	VAL
1	D	468	CYS
1	D	469	THR
1	D	483	PHE
1	D	495	LEU
1	D	499	LEU
1	D	510	ILE
1	D	521	ARG
1	D	527	THR
1	D	530	ASN
1	D	532	HIS
1	D	538	TYR
1	D	544	ASP
1	D	560	SER
1	D	564	ASP
1	D	570	THR
1	D	573	LEU
1	D	576	ASP
1	D	577	CYS
1	D	613	PRO
1	D	620	LEU
1	D	647	THR
1	D	650	ASP
1	D	672	VAL
1	D	675	THR
1	D	689	ASP
1	D	727	LEU
1	D	728	LEU
1	D	731	THR
1	D	740	SER
1	D	741	LYS
1	D	742	GLN
1	D	750	SER
1	D	756	ARG
1	D	780	GLU
1	D	801	LEU
1	D	804	LEU
1	D	808	MET
1	D	817	ASP
1	D	839	LEU

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Mol	Chain	Res	Type
1	D	840	THR
1	D	861	GLU
1	D	877	THR
1	D	916	PRO
1	D	926	THR
1	D	949	VAL
1	D	951	GLN
1	D	981	LEU
1	D	985	LEU
1	D	998	LYS
1	D	1003	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	31	GLN
1	A	196	HIS
1	A	202	GLN
1	A	397	HIS
1	A	463	GLN
1	A	478	HIS
1	A	555	HIS
1	A	684	HIS
1	A	709	ASN
1	B	202	GLN
1	B	310	ASN
1	B	463	GLN
1	B	555	HIS
1	B	963	GLN
1	C	58	HIS
1	C	202	GLN
1	C	295	GLN
1	C	417	GLN
1	C	463	GLN
1	D	202	GLN
1	D	417	GLN
1	D	447	GLN
1	D	463	GLN
1	D	555	HIS

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	924/1034 (89%)	-0.00	42 (4%) 37 23	11, 21, 94, 177	0
1	B	922/1034 (89%)	0.34	100 (10%) 8 4	9, 25, 146, 228	0
1	C	922/1034 (89%)	1.16	185 (20%) 1 1	25, 71, 152, 347	0
1	D	922/1034 (89%)	1.55	229 (24%) 1 1	24, 71, 221, 430	0
All	All	3690/4136 (89%)	0.76	556 (15%) 3 2	9, 53, 158, 430	0

All (556) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	823	HIS	21.6
1	D	936	THR	18.8
1	D	955	ALA	18.5
1	D	940	ALA	16.8
1	D	935	SER	16.2
1	C	46	LEU	15.7
1	B	894	PRO	15.7
1	D	953	ALA	15.7
1	C	111	THR	15.6
1	D	951	GLN	15.2
1	D	838	ALA	15.0
1	D	91	VAL	14.6
1	D	837	LYS	14.6
1	D	954	GLY	14.0
1	B	893	GLU	13.9
1	D	894	PRO	13.5
1	D	824	SER	13.2
1	D	950	TRP	12.9
1	D	930	ALA	12.5
1	D	829	LEU	12.5
1	D	97	PHE	12.4

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Mol	Chain	Res	Type	RSRZ
1	D	937	ALA	12.4
1	D	808	MET	12.1
1	C	110	LEU	12.1
1	B	836	PHE	11.7
1	D	836	PHE	11.6
1	D	948	PHE	11.3
1	D	835	ASN	11.3
1	C	48	LEU	11.0
1	D	481	VAL	11.0
1	D	952	MET	10.8
1	D	834	GLU	10.6
1	B	847	ARG	10.6
1	D	934	ALA	10.5
1	C	93	ARG	10.5
1	D	931	LEU	10.2
1	C	40	TRP	10.2
1	C	966	SER	10.2
1	D	44	ALA	10.1
1	C	45	PRO	10.1
1	D	90	ASP	9.7
1	C	77	SER	9.7
1	D	43	ALA	9.6
1	C	200	GLY	9.4
1	C	73	SER	9.4
1	C	113	ASN	9.1
1	D	45	PRO	8.9
1	D	811	SER	8.8
1	C	52	LEU	8.7
1	B	484	LEU	8.7
1	B	837	LYS	8.5
1	B	922	GLY	8.5
1	C	78	ASP	8.4
1	B	848	ALA	8.4
1	B	951	GLN	8.4
1	B	934	ALA	8.3
1	C	76	THR	8.2
1	D	825	TRP	8.2
1	B	885	LEU	8.1
1	D	413	ALA	8.1
1	D	810	ALA	8.1
1	C	988	ALA	8.0
1	D	466	ASN	8.0

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Mol	Chain	Res	Type	RSRZ
1	D	828	ASP	8.0
1	C	55	ILE	7.8
1	C	112	GLY	7.8
1	B	884	GLN	7.8
1	B	937	ALA	7.8
1	D	492	GLY	7.7
1	D	821	ALA	7.7
1	D	841	ALA	7.6
1	D	493	GLU	7.5
1	B	829	LEU	7.5
1	B	838	ALA	7.5
1	A	83	TRP	7.3
1	C	178	ILE	7.3
1	D	945	ASN	7.3
1	C	460	GLN	7.2
1	C	35	PRO	7.2
1	C	50	TRP	7.1
1	D	509	TYR	7.0
1	C	301	THR	6.9
1	D	800	GLU	6.8
1	D	473	SER	6.6
1	D	947	LYS	6.6
1	D	480	GLN	6.6
1	A	77	SER	6.5
1	D	531	ILE	6.5
1	D	141	ASP	6.5
1	D	77	SER	6.5
1	D	37	PHE	6.4
1	C	47	ALA	6.4
1	A	179	LEU	6.3
1	D	932	LEU	6.3
1	D	819	ASP	6.3
1	D	839	LEU	6.2
1	A	176	PRO	6.1
1	C	97	PHE	6.1
1	C	34	TRP	6.1
1	A	975	SER	6.0
1	D	89	LEU	6.0
1	D	956	GLN	6.0
1	D	893	GLU	6.0
1	D	76	THR	6.0
1	D	179	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	804	LEU	5.9
1	D	488	PRO	5.9
1	D	142	MET	5.9
1	B	888	LYS	5.9
1	C	49	ALA	5.8
1	D	182	GLY	5.8
1	D	942	TYR	5.7
1	C	79	MET	5.7
1	C	105	ALA	5.5
1	C	199	VAL	5.5
1	D	938	PHE	5.4
1	C	843	SER	5.4
1	D	139	LEU	5.4
1	D	530	ASN	5.4
1	B	517	LEU	5.4
1	A	107	ALA	5.3
1	C	201	ARG	5.3
1	D	916	PRO	5.2
1	C	195	PRO	5.1
1	D	186	GLN	5.1
1	D	479	GLY	5.1
1	D	83	TRP	5.1
1	B	824	SER	5.1
1	C	186	GLN	5.1
1	A	47	ALA	5.0
1	D	92	PHE	5.0
1	C	96	SER	5.0
1	D	946	PRO	5.0
1	A	108	ALA	5.0
1	C	107	ALA	5.0
1	A	59	CYS	5.0
1	B	864	TRP	4.9
1	C	92	PHE	4.9
1	D	860	VAL	4.9
1	D	865	LYS	4.9
1	D	504	ASP	4.9
1	D	277	LEU	4.9
1	D	526	ARG	4.9
1	B	952	MET	4.9
1	D	501	SER	4.9
1	B	892	ILE	4.9
1	D	941	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	82	LEU	4.8
1	A	181	ASP	4.8
1	C	701	PRO	4.8
1	C	818	ASP	4.8
1	B	909	THR	4.8
1	D	468	CYS	4.7
1	C	369	ASP	4.7
1	C	589	PRO	4.7
1	A	97	PHE	4.7
1	D	507	GLN	4.7
1	C	817	ASP	4.7
1	C	676	GLY	4.7
1	D	181	ASP	4.7
1	D	661	LEU	4.6
1	C	432	MET	4.6
1	D	472	ARG	4.6
1	D	145	LEU	4.6
1	C	244	PHE	4.5
1	C	41	LEU	4.5
1	D	178	ILE	4.5
1	D	822	ALA	4.5
1	D	887	ALA	4.5
1	D	1003	ARG	4.5
1	D	144	PRO	4.5
1	C	61	VAL	4.5
1	B	938	PHE	4.5
1	D	863	GLU	4.5
1	D	807	VAL	4.5
1	C	323	ALA	4.4
1	D	939	LYS	4.4
1	C	394	ASP	4.4
1	C	56	CYS	4.4
1	C	82	LEU	4.4
1	C	242	HIS	4.4
1	A	922	GLY	4.4
1	C	205	ALA	4.4
1	C	99	GLU	4.4
1	C	921	ARG	4.3
1	C	166	LEU	4.3
1	D	500	ASN	4.3
1	D	412	ALA	4.3
1	C	1002	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	833	PHE	4.3
1	D	140	LEU	4.3
1	D	926	THR	4.3
1	D	496	SER	4.3
1	A	175	ALA	4.3
1	B	820	ALA	4.3
1	B	846	LEU	4.2
1	B	497	PHE	4.2
1	C	840	THR	4.2
1	A	61	VAL	4.2
1	C	837	LYS	4.2
1	B	955	ALA	4.2
1	D	662	GLY	4.2
1	D	885	LEU	4.1
1	C	810	ALA	4.1
1	D	180	LYS	4.1
1	D	31	GLN	4.1
1	D	28	ALA	4.1
1	B	890	CYS	4.1
1	B	857	LEU	4.1
1	C	476	VAL	4.0
1	D	826	ASP	4.0
1	B	845	SER	4.0
1	D	96	SER	4.0
1	B	83	TRP	3.9
1	B	810	ALA	3.9
1	B	887	ALA	3.9
1	D	866	VAL	3.9
1	D	913	LEU	3.9
1	C	59	CYS	3.9
1	D	490	ASN	3.9
1	D	668	PHE	3.9
1	D	914	GLU	3.9
1	B	891	ALA	3.8
1	D	966	SER	3.8
1	C	827	PRO	3.8
1	D	335	SER	3.8
1	A	78	ASP	3.8
1	C	932	LEU	3.8
1	C	504	ASP	3.8
1	D	957	LEU	3.8
1	D	47	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	560	SER	3.8
1	D	34	TRP	3.7
1	D	963	GLN	3.7
1	D	74	TRP	3.7
1	C	481	VAL	3.7
1	D	56	CYS	3.7
1	C	27	TYR	3.7
1	C	85	SER	3.7
1	D	917	PHE	3.7
1	C	472	ARG	3.7
1	B	830	ALA	3.7
1	C	138	PHE	3.7
1	A	52	LEU	3.6
1	D	912	LEU	3.6
1	C	809	GLN	3.6
1	D	806	LYS	3.6
1	D	886	HIS	3.6
1	A	66	PRO	3.6
1	A	178	ILE	3.6
1	D	944	THR	3.6
1	A	55	ILE	3.6
1	B	947	LYS	3.5
1	B	507	GLN	3.5
1	B	914	GLU	3.5
1	A	818	ASP	3.5
1	C	808	MET	3.5
1	B	877	THR	3.5
1	D	850	LEU	3.5
1	B	921	ARG	3.5
1	C	516	ASP	3.5
1	B	136	PRO	3.5
1	A	180	LYS	3.5
1	A	62	ASP	3.5
1	C	304	THR	3.5
1	C	100	ARG	3.5
1	B	945	ASN	3.4
1	C	114	PHE	3.4
1	A	79	MET	3.4
1	D	464	TRP	3.4
1	C	108	ALA	3.4
1	D	494	VAL	3.4
1	C	545	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	45	PRO	3.4
1	C	346	LEU	3.4
1	D	392	ASP	3.4
1	D	489	GLU	3.4
1	D	644	GLU	3.4
1	B	913	LEU	3.4
1	C	53	THR	3.4
1	D	35	PRO	3.4
1	C	820	ALA	3.4
1	D	878	TYR	3.4
1	D	476	VAL	3.3
1	D	809	GLN	3.3
1	B	879	PRO	3.3
1	D	852	ALA	3.3
1	B	809	GLN	3.3
1	D	801	LEU	3.3
1	D	65	ASP	3.3
1	C	57	LEU	3.3
1	B	839	LEU	3.3
1	D	183	GLY	3.3
1	C	204	GLN	3.3
1	D	184	ALA	3.3
1	B	41	LEU	3.3
1	D	469	THR	3.3
1	A	99	GLU	3.3
1	C	723	ASP	3.3
1	C	264	ARG	3.3
1	D	587	HIS	3.3
1	C	130	ASN	3.2
1	C	126	SER	3.2
1	B	63	LEU	3.2
1	C	989	GLY	3.2
1	D	450	SER	3.2
1	B	835	ASN	3.2
1	A	976	ASP	3.2
1	C	371	ALA	3.2
1	D	769	ALA	3.2
1	B	948	PHE	3.2
1	D	50	TRP	3.1
1	B	856	ALA	3.1
1	D	984	PRO	3.1
1	C	94	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	882	VAL	3.1
1	C	54	ARG	3.1
1	D	525	LEU	3.1
1	B	956	GLN	3.1
1	D	882	VAL	3.1
1	A	974	GLY	3.1
1	D	960	ILE	3.1
1	D	175	ALA	3.1
1	B	58	HIS	3.1
1	C	700	GLN	3.0
1	D	849	VAL	3.0
1	C	38	PRO	3.0
1	D	308	GLU	3.0
1	A	811	SER	3.0
1	D	78	ASP	3.0
1	C	66	PRO	3.0
1	D	276	LEU	3.0
1	D	857	LEU	3.0
1	B	135	GLY	3.0
1	D	187	VAL	3.0
1	A	819	ASP	3.0
1	D	73	SER	3.0
1	C	279	LEU	3.0
1	D	856	ALA	3.0
1	D	910	ALA	3.0
1	C	305	VAL	3.0
1	B	863	GLU	3.0
1	C	927	SER	2.9
1	B	936	THR	2.9
1	C	847	ARG	2.9
1	D	169	SER	2.9
1	C	585	PRO	2.9
1	B	958	ALA	2.9
1	C	975	SER	2.9
1	D	38	PRO	2.9
1	C	859	ALA	2.9
1	A	98	PRO	2.9
1	B	482	PRO	2.9
1	D	411	PRO	2.9
1	D	199	VAL	2.9
1	D	497	PHE	2.9
1	B	886	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	131	PRO	2.9
1	B	911	ALA	2.9
1	B	858	GLY	2.8
1	C	335	SER	2.8
1	C	300	LYS	2.8
1	C	145	LEU	2.8
1	D	719	ASN	2.8
1	D	979	PRO	2.8
1	B	851	GLU	2.8
1	C	1001	LEU	2.8
1	B	841	ALA	2.8
1	C	324	GLY	2.8
1	D	88	GLN	2.8
1	D	520	GLN	2.8
1	C	36	LYS	2.8
1	D	467	GLU	2.8
1	D	820	ALA	2.8
1	B	826	ASP	2.8
1	B	118	GLY	2.8
1	D	417	GLN	2.7
1	B	865	LYS	2.7
1	C	81	ALA	2.7
1	C	987	TYR	2.7
1	C	944	THR	2.7
1	B	876	LEU	2.7
1	D	558	PHE	2.7
1	D	423	GLU	2.7
1	A	67	THR	2.7
1	C	307	PHE	2.7
1	D	768	PRO	2.7
1	B	920	ASP	2.7
1	D	962	ALA	2.7
1	C	362	ALA	2.7
1	D	350	ASP	2.7
1	C	520	GLN	2.7
1	B	227	LYS	2.7
1	B	134	THR	2.7
1	B	910	ALA	2.7
1	C	117	ARG	2.7
1	D	176	PRO	2.7
1	D	478	HIS	2.7
1	B	840	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	149	GLU	2.7
1	B	518	GLN	2.6
1	C	265	ALA	2.6
1	C	322	PRO	2.6
1	C	179	LEU	2.6
1	A	65	ASP	2.6
1	D	113	ASN	2.6
1	B	64	GLU	2.6
1	C	391	ASP	2.6
1	C	393	ALA	2.6
1	D	660	TYR	2.6
1	D	929	TRP	2.6
1	B	817	ASP	2.6
1	C	517	LEU	2.6
1	D	33	ILE	2.6
1	D	414	LEU	2.6
1	D	482	PRO	2.6
1	C	75	ALA	2.6
1	C	680	ALA	2.6
1	C	807	VAL	2.5
1	C	433	ARG	2.5
1	C	779	GLY	2.5
1	A	177	SER	2.5
1	B	932	LEU	2.5
1	D	508	LYS	2.5
1	B	514	ALA	2.5
1	A	977	GLY	2.5
1	D	718	ASN	2.5
1	C	722	SER	2.5
1	C	282	ASN	2.5
1	D	30	LEU	2.5
1	D	310	ASN	2.5
1	D	112	GLY	2.5
1	B	111	THR	2.5
1	D	958	ALA	2.5
1	D	920	ASP	2.5
1	D	353	SER	2.5
1	D	483	PHE	2.5
1	B	510	ILE	2.5
1	C	274	ASP	2.5
1	B	950	TRP	2.4
1	B	72	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	51	GLU	2.4
1	D	598	VAL	2.4
1	B	263	THR	2.4
1	C	602	GLN	2.4
1	C	299	SER	2.4
1	D	52	LEU	2.4
1	C	640	PRO	2.4
1	C	127	LEU	2.4
1	C	80	ALA	2.4
1	C	155	ARG	2.4
1	D	701	PRO	2.4
1	D	862	HIS	2.4
1	C	136	PRO	2.4
1	D	104	GLU	2.4
1	B	57	LEU	2.4
1	D	595	VAL	2.4
1	C	193	GLU	2.4
1	D	134	THR	2.4
1	C	198	LEU	2.4
1	C	798	ASP	2.4
1	A	676	GLY	2.4
1	C	26	VAL	2.4
1	D	614	ALA	2.4
1	C	858	GLY	2.3
1	C	681	ALA	2.3
1	C	856	ALA	2.3
1	A	54	ARG	2.3
1	B	478	HIS	2.3
1	D	333	ARG	2.3
1	D	513	LEU	2.3
1	D	46	LEU	2.3
1	C	203	TRP	2.3
1	C	738	ASP	2.3
1	D	111	THR	2.3
1	D	210	ASP	2.3
1	C	314	HIS	2.3
1	D	602	GLN	2.3
1	C	62	ASP	2.3
1	D	151	CYS	2.3
1	C	104	GLU	2.3
1	B	825	TRP	2.3
1	C	957	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	907	ALA	2.3
1	C	118	GLY	2.3
1	D	390	CYS	2.3
1	C	543	VAL	2.3
1	C	133	LYS	2.3
1	C	689	ASP	2.3
1	D	470	ASN	2.3
1	B	248	PRO	2.2
1	C	668	PHE	2.2
1	C	378	TRP	2.2
1	C	243	ASP	2.2
1	D	105	ALA	2.2
1	B	483	PHE	2.2
1	D	588	PHE	2.2
1	D	855	ASN	2.2
1	C	43	ALA	2.2
1	D	978	MET	2.2
1	A	136	PRO	2.2
1	A	48	LEU	2.2
1	C	503	PHE	2.2
1	C	32	ASN	2.2
1	D	983	THR	2.2
1	C	74	TRP	2.2
1	C	475	ARG	2.2
1	C	182	GLY	2.2
1	A	58	HIS	2.2
1	C	327	MET	2.2
1	B	781	PRO	2.2
1	D	64	GLU	2.2
1	B	935	SER	2.2
1	D	26	VAL	2.2
1	D	645	ASN	2.2
1	C	845	SER	2.1
1	B	42	HIS	2.1
1	C	192	THR	2.1
1	A	809	GLN	2.1
1	B	503	PHE	2.1
1	C	841	ALA	2.1
1	C	917	PHE	2.1
1	D	840	THR	2.1
1	C	202	GLN	2.1
1	C	125	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	838	ALA	2.1
1	B	130	ASN	2.1
1	C	154	THR	2.1
1	D	53	THR	2.1
1	C	641	ASP	2.1
1	D	75	ALA	2.1
1	D	460	GLN	2.1
1	D	463	GLN	2.1
1	B	59	CYS	2.1
1	C	720	SER	2.1
1	C	811	SER	2.1
1	C	1000	TYR	2.1
1	B	477	ARG	2.1
1	C	184	ALA	2.1
1	B	804	LEU	2.1
1	B	929	TRP	2.1
1	C	42	HIS	2.1
1	C	281	GLN	2.1
1	C	918	LEU	2.1
1	C	474	GLU	2.0
1	A	810	ALA	2.0
1	D	57	LEU	2.0
1	C	537	ALA	2.0
1	D	928	TYR	2.0
1	C	196	HIS	2.0
1	C	321	SER	2.0
1	B	764	SER	2.0
1	D	512	ASP	2.0
1	D	94	GLY	2.0
1	B	22	GLN	2.0
1	D	278	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.