



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:14 PM EDT

PDB ID : 3MDJ
Title : ER Aminopeptidase, ERAP1, Bound to the Zinc Aminopeptidase Inhibitor, Bestatin
Authors : Nguyen, T.T.; Stern, L.J.
Deposited on : unknown
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

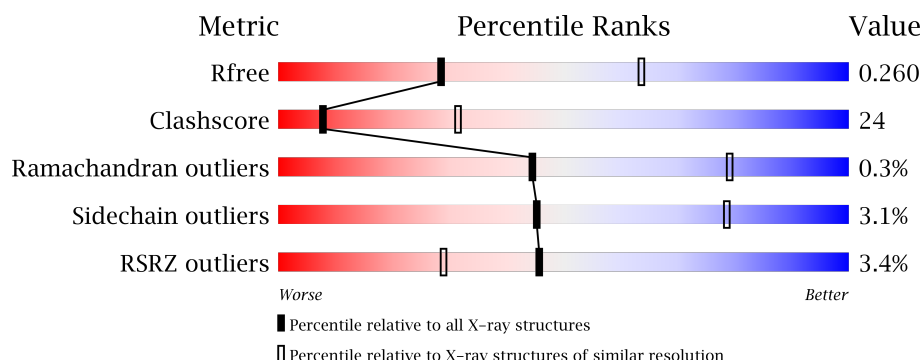
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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	921	<div> <div>2%</div> <div> <div>51%</div> <div>36%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	921	<div> <div>4%</div> <div> <div>54%</div> <div>33%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	921	<div> <div>3%</div> <div> <div>50%</div> <div>38%</div> <div>•</div> <div>11%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BES	A	1001	-	-	-	X
3	BES	B	1001	-	-	X	X
3	BES	C	1001	-	-	-	X
4	NAG	A	6001	X	-	-	-
4	NAG	C	5001	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20163 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	818	Total	C	N	O	S	55	0	0
			6625	4271	1096	1227	31			
1	B	821	Total	C	N	O	S	50	0	0
			6643	4281	1099	1232	31			
1	C	819	Total	C	N	O	S	68	0	0
			6634	4276	1097	1230	31			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08
A	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
A	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
A	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
A	940	HIS	-	EXPRESSION TAG	UNP Q9NZ08
A	941	ASP	-	EXPRESSION TAG	UNP Q9NZ08
A	942	PRO	-	EXPRESSION TAG	UNP Q9NZ08
A	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	944	ALA	-	EXPRESSION TAG	UNP Q9NZ08
A	945	ASP	-	EXPRESSION TAG	UNP Q9NZ08
A	946	ALA	-	EXPRESSION TAG	UNP Q9NZ08
A	947	THR	-	EXPRESSION TAG	UNP Q9NZ08
A	948	GLY	-	EXPRESSION TAG	UNP Q9NZ08
A	949	LEU	-	EXPRESSION TAG	UNP Q9NZ08
A	950	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	951	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	952	MET	-	EXPRESSION TAG	UNP Q9NZ08
A	953	LEU	-	EXPRESSION TAG	UNP Q9NZ08
A	954	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	955	SER	-	EXPRESSION TAG	UNP Q9NZ08
A	956	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08
B	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
B	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
B	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
B	940	HIS	-	EXPRESSION TAG	UNP Q9NZ08
B	941	ASP	-	EXPRESSION TAG	UNP Q9NZ08
B	942	PRO	-	EXPRESSION TAG	UNP Q9NZ08
B	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	944	ALA	-	EXPRESSION TAG	UNP Q9NZ08
B	945	ASP	-	EXPRESSION TAG	UNP Q9NZ08
B	946	ALA	-	EXPRESSION TAG	UNP Q9NZ08
B	947	THR	-	EXPRESSION TAG	UNP Q9NZ08
B	948	GLY	-	EXPRESSION TAG	UNP Q9NZ08
B	949	LEU	-	EXPRESSION TAG	UNP Q9NZ08
B	950	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	951	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	952	MET	-	EXPRESSION TAG	UNP Q9NZ08
B	953	LEU	-	EXPRESSION TAG	UNP Q9NZ08
B	954	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	955	SER	-	EXPRESSION TAG	UNP Q9NZ08
B	956	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08
C	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08
C	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
C	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
C	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
C	940	HIS	-	EXPRESSION TAG	UNP Q9NZ08
C	941	ASP	-	EXPRESSION TAG	UNP Q9NZ08
C	942	PRO	-	EXPRESSION TAG	UNP Q9NZ08
C	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	944	ALA	-	EXPRESSION TAG	UNP Q9NZ08
C	945	ASP	-	EXPRESSION TAG	UNP Q9NZ08
C	946	ALA	-	EXPRESSION TAG	UNP Q9NZ08
C	947	THR	-	EXPRESSION TAG	UNP Q9NZ08
C	948	GLY	-	EXPRESSION TAG	UNP Q9NZ08
C	949	LEU	-	EXPRESSION TAG	UNP Q9NZ08
C	950	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	951	ARG	-	EXPRESSION TAG	UNP Q9NZ08
C	952	MET	-	EXPRESSION TAG	UNP Q9NZ08
C	953	LEU	-	EXPRESSION TAG	UNP Q9NZ08
C	954	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	955	SER	-	EXPRESSION TAG	UNP Q9NZ08
C	956	ARG	-	EXPRESSION TAG	UNP Q9NZ08

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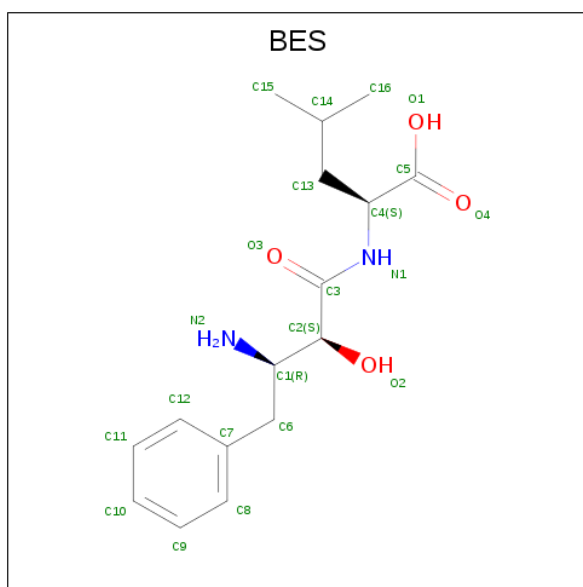
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Chain	Residue	Modelled	Actual	Comment	Reference
C	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: $C_{16}H_{24}N_2O_4$).



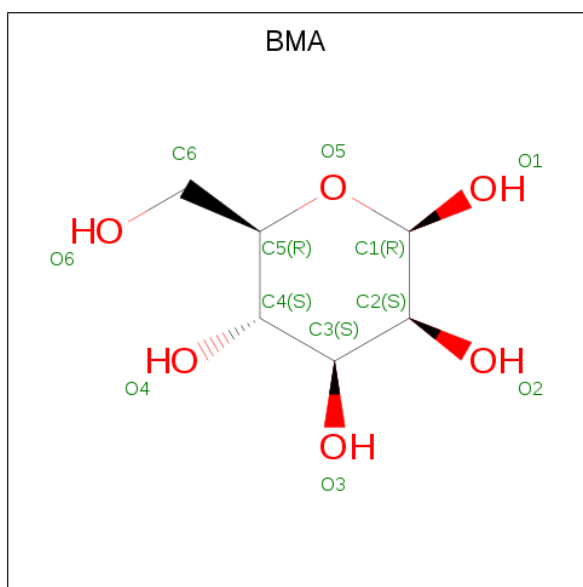
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 22	C 16	N 2	O 4	0	0
3	B	1	Total 22	C 16	N 2	O 4	0	0
3	C	1	Total 22	C 16	N 2	O 4	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



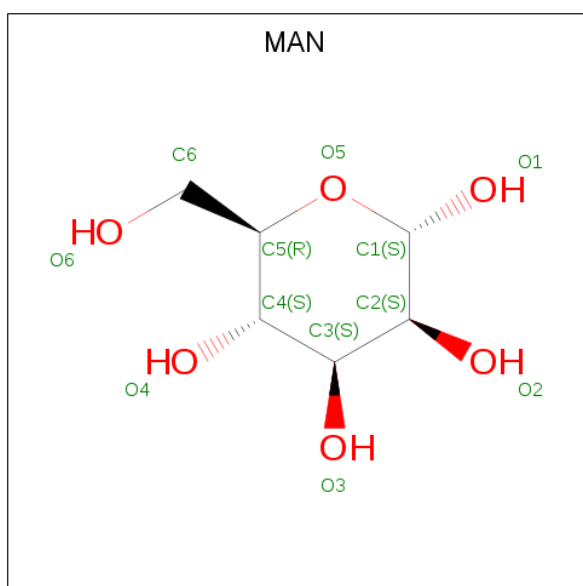
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

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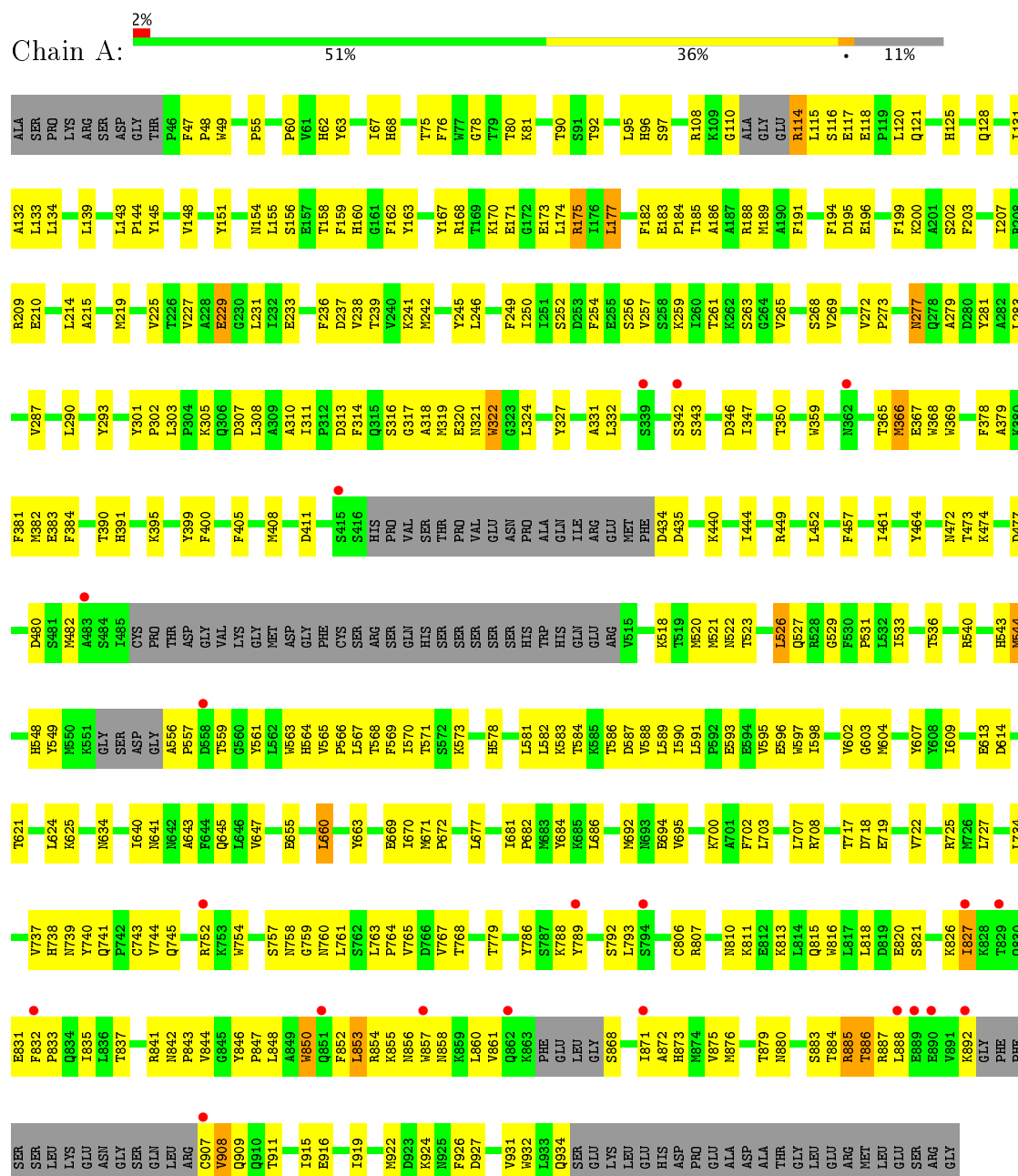
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		

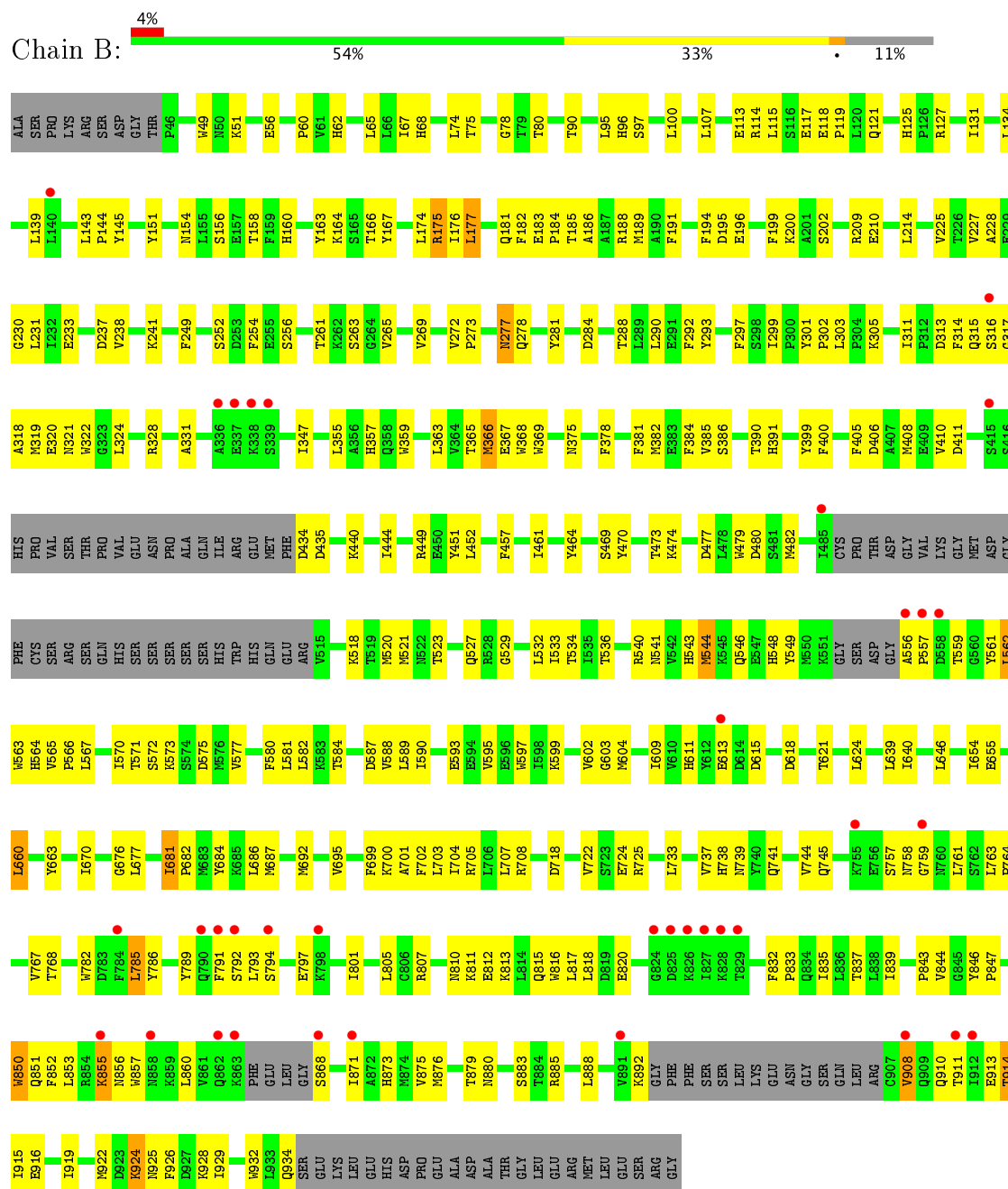
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

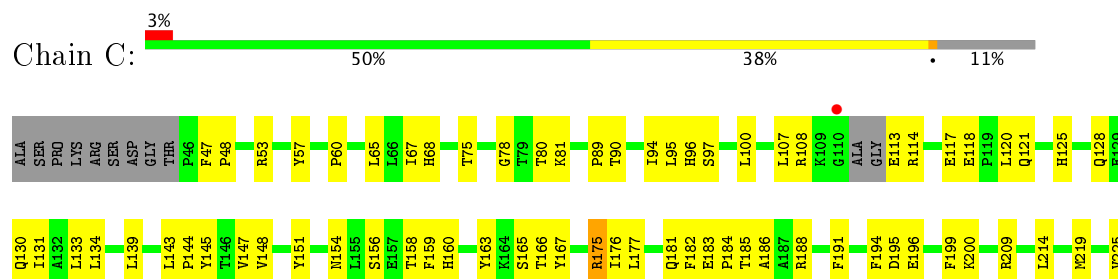
- Molecule 1: Endoplasmic reticulum aminopeptidase 1



- Molecule 1: Endoplasmic reticulum aminopeptidase 1



- Molecule 1: Endoplasmic reticulum aminopeptidase 1



LYS	S869	S795	L707	D614	K545	W479	V396	W322	T236
LEU	S870	T796	L710	D615	Q546	D480	V399	G323	V227
HIS	I871	E547	L711	G616	E548	S481	F400	T324	A228
ASP	H873	I801	T717	D617	E549	N482	F405	T325	E229
PRO	H874	E802	T718	D618	K550	L485	M408	T326	G230
GLU	N875	F803	D718	D619	K551	CYS	F408	Y327	L231
ALA	N876	A804	E719	L620	GLY	PRO	M409	R328	T232
ASP	T879	L805	L727	T621	ASP	THR	D411	A331	E233
ALA	N880	R806	L731	L624	ASP	GLY	A412	L332	D237
THR	N881	R807	L732	K625	ASP	GLY	A413	L333	V238
GLY	N882	L810	L733	L626	ASP	GLY	A414	F334	T239
LEU	S883	N811	L734	L627	P557	LYS	S415	E337	W240
GLU	T884	K812	L735	L628	E558	GLY	S416	R338	K241
ARG	R885	K813	L736	L629	T559	MET	HIS	K339	F249
MET	T886	F813	L737	I640	ASP	ASP	PRO	S343	S252
LEU	R887	W816	L738	I641	Y561	GLY	VAL	K344	D263
GLU	L888	A735	L739	L642	E564	THR	SER	L345	F254
ARG	K892	E820	L740	L643	V565	CYS	THR	L346	K259
GLY	GLY	G824	L741	L644	P566	ARG	VAL	I347	T260
PHE	PHE	D825	L742	L645	L567	SER	GLN	T348	K261
SER	SER	K826	L743	L646	I570	HIS	ASN	K349	T262
LEU	LEU	I827	L744	L647	T571	SER	PRO	T350	K263
LYS	LYS	K828	L745	L648	S572	SER	ALA	L355	S264
GLU	GLU	T829	L746	L649	S573	SER	ILE	A356	G264
ASN	ASN	K830	L747	L650	S574	SER	ARG	R357	V265
GLY	GLY	E831	L748	L651	D575	SER	GLU	V269	V269
SER	SER	F832	L749	L652	M576	TRP	MET	N362	N277
GLN	GLN	K833	L750	L653	V577	HIS	PHE	L363	Q278
LEU	LEU	E834	L751	L654	F580	GLN	D434	V364	A279
ARG	ARG	I835	L752	L655	L581	GLU	D435	T365	N280
C907	C907	L836	L753	L656	L582	ARG	V436	N366	D280
V908	V908	T837	L754	L657	K583	V515	Y438	E367	Y281
Q909	Q909	W844	L755	L658	T584	K518	D439	K368	K286
Q910	Q910	G845	L756	L659	E585	T519	K440	N370	V287
T911	T911	Y846	L757	L660	T586	N520	I444	D371	L290
E912	E912	P847	L758	L661	D587	N521	L452	L372	E291
E913	E913	L850	L759	L662	V588	N522	R449	W373	F292
T914	T914	W850	L760	L663	L589	N524	L453	L374	Y293
I915	I915	Q851	L761	L664	I590	N525	L454	N375	L303
E916	E916	F852	L762	L665	L591	L526	F457	A379	F304
I919	I919	L853	L763	L666	V595	N529	K380	K381	K305
N922	N922	K854	L764	L667	E596	F530	I461	N382	A310
D923	D923	N855	L765	L668	W597	N533	Y464	E383	D313
K924	K924	W857	L766	L669	N601	T534	Y470	F384	F314
N925	N925	L860	L767	L670	N602	T535	Y471	V385	Q315
F926	F926	V861	L768	L671	G603	T536	T473	S386	S316
I929	I929	Q862	L769	L672	N604	V537	K474	V387	G317
W932	W932	K863	L770	L673	A701	N540	M475	T390	A318
L933	L933	PHE	L771	L674	L702	N541	E476	R391	R319
Q934	Q934	GLU	L772	L675	L703	N542	D477	E320	E320
SER	SER	LEU	L773	L676	L704	N543	L478	K395	N321
GLU	GLU	GLY	L774	L677	L705	N544			
		S868	L775	L678	L706				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.03 Å 234.63 Å 95.86 Å 90.00° 103.59° 90.00°	Depositor
Resolution (Å)	38.11 – 2.95 38.11 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.11-2.95) 99.8 (38.11-2.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.95 Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.199 , 0.264 0.193 , 0.260	Depositor DCC
R_{free} test set	3206 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20163	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, 0.333 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: BES, ZN, BMA, NAG, MAN

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	0.27	0/6785	0.45	0/9195
1	B	0.28	0/6804	0.46	0/9222
1	C	0.27	0/6794	0.45	0/9207
All	All	0.27	0/20383	0.45	0/27624

There are no bond length outliers.

There are no bond angle outliers.

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	6625	0	6567	327	0
1	B	6643	0	6582	315	0
1	C	6634	0	6574	322	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	0	22	2	0
3	B	22	0	22	10	0
3	C	22	0	23	6	0
4	A	56	0	50	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	42	0	38	1	0
4	C	28	0	24	1	0
5	A	11	0	8	0	0
5	C	11	0	8	0	0
6	A	22	0	20	1	0
6	C	22	0	20	1	0
All	All	20163	0	19958	955	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 24.

All (955) 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:C:640:ILE:HD11	1:C:663:TYR:HE2	1.13	1.12
1:B:113:GLU:O	1:B:117:GLU:HG3	1.49	1.12
1:A:210:GLU:HG3	4:A:5001:NAG:H83	1.37	1.07
1:A:875:VAL:HG11	1:A:908:VAL:CG2	1.86	1.04
1:C:319:MET:HE1	3:C:1001:BES:HN21	1.23	1.03
1:C:640:ILE:HD11	1:C:663:TYR:CE2	1.95	1.02
1:B:320:GLU:OE1	3:B:1001:BES:N2	1.93	1.01
1:A:571:THR:HG22	1:A:573:LYS:H	1.21	1.01
1:A:588:VAL:HG11	1:B:241:LYS:HD2	1.42	1.00
1:A:737:VAL:HG13	1:A:807:ARG:HH21	1.24	1.00
1:B:621:THR:HG22	1:B:660:LEU:HG	1.41	0.99
1:C:314:PHE:CE2	1:C:316:SER:HB2	1.97	0.99
1:C:143:LEU:HD12	1:C:144:PRO:HD2	1.43	0.99
1:A:875:VAL:HG11	1:A:908:VAL:HG21	1.41	0.99
1:B:318:ALA:O	3:B:1001:BES:H61	1.63	0.99
1:A:210:GLU:HG3	4:A:5001:NAG:C8	1.92	0.99
1:C:621:THR:HG22	1:C:660:LEU:HD13	1.43	0.99
1:C:68:HIS:HE1	1:C:231:LEU:HD21	1.28	0.98
1:C:113:GLU:HG2	1:C:114:ARG:H	1.22	0.98
1:A:143:LEU:HD12	1:A:144:PRO:HD2	1.45	0.97
1:B:143:LEU:HD12	1:B:144:PRO:HD2	1.46	0.96
1:B:314:PHE:CE2	1:B:316:SER:HB2	2.01	0.94
1:B:544:MET:HG3	1:B:582:LEU:HD23	1.50	0.93
1:C:227:VAL:HG21	1:C:233:GLU:HB2	1.50	0.93
1:B:261:THR:HG22	1:B:265:VAL:H	1.32	0.92
1:A:533:ILE:HD13	1:A:567:LEU:HD21	1.51	0.92
1:B:737:VAL:HG13	1:B:807:ARG:HH21	1.31	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:TYR:CE1	1:B:609:ILE:HD11	2.06	0.91
1:C:108:ARG:HG2	1:C:117:GLU:HG2	1.52	0.90
1:B:121:GLN:HB3	1:B:134:LEU:HB2	1.57	0.87
1:B:856:ASN:O	1:B:860:LEU:HB2	1.74	0.87
1:A:60:PRO:HG3	1:A:194:PHE:CD2	2.11	0.86
1:A:737:VAL:HG13	1:A:807:ARG:NH2	1.90	0.86
1:B:763:LEU:HG	1:B:768:THR:HG22	1.59	0.84
1:A:621:THR:HG22	1:A:660:LEU:HG	1.60	0.84
1:B:185:THR:HG23	1:B:188:ARG:CZ	2.07	0.83
1:C:810:ASN:HD22	1:C:813:LYS:HD3	1.44	0.83
1:A:227:VAL:HG21	1:A:233:GLU:HB2	1.59	0.83
1:B:316:SER:HB3	3:B:1001:BES:H8	1.62	0.82
1:A:314:PHE:CE2	1:A:316:SER:HB2	2.14	0.82
1:B:182:PHE:HA	1:B:186:ALA:HB3	1.58	0.82
1:C:544:MET:SD	1:C:582:LEU:HD23	2.19	0.82
1:C:182:PHE:HA	1:C:186:ALA:HB3	1.62	0.81
1:A:96:HIS:HD2	1:A:195:ASP:H	1.27	0.81
1:C:314:PHE:HE2	1:C:316:SER:HB2	1.44	0.81
1:A:121:GLN:HB3	1:A:134:LEU:HB2	1.62	0.80
1:A:381:PHE:HZ	1:A:449:ARG:HD2	1.46	0.80
1:A:763:LEU:HG	1:A:768:THR:HG22	1.63	0.80
1:A:872:ALA:O	1:A:875:VAL:HG12	1.81	0.80
1:C:621:THR:HG22	1:C:660:LEU:CD1	2.10	0.80
1:A:182:PHE:HA	1:A:186:ALA:HB3	1.64	0.80
1:C:570:ILE:HG23	1:C:602:VAL:HG21	1.64	0.80
1:C:60:PRO:HG3	1:C:194:PHE:CD2	2.16	0.79
1:B:473:THR:HG23	1:B:477:ASP:HB2	1.64	0.79
1:B:875:VAL:CG1	1:B:908:VAL:HG11	2.12	0.79
1:A:473:THR:HG23	1:A:477:ASP:HB2	1.64	0.79
1:A:681:ILE:HA	1:A:684:TYR:CE2	2.17	0.78
1:C:875:VAL:CG1	1:C:908:VAL:HG11	2.12	0.78
1:C:113:GLU:HG2	1:C:114:ARG:N	1.97	0.78
1:B:621:THR:HG22	1:B:660:LEU:CG	2.13	0.78
1:A:80:THR:HG23	1:A:151:TYR:HE1	1.47	0.78
1:B:536:THR:OG1	1:B:613:GLU:HG3	1.84	0.77
1:C:261:THR:HG23	1:C:263:SER:H	1.48	0.77
1:C:473:THR:HG23	1:C:477:ASP:HB2	1.65	0.77
1:A:350:THR:HA	3:A:1001:BES:H162	1.66	0.77
1:B:883:SER:HB2	1:B:922:MET:HG3	1.67	0.77
1:A:90:THR:HG22	1:A:92:THR:H	1.50	0.77
1:C:571:THR:HG22	1:C:573:LYS:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:HG22	1:A:154:ASN:OD1	1.85	0.76
1:B:261:THR:HG23	1:B:263:SER:H	1.50	0.76
1:C:316:SER:H	1:C:317:GLY:HA2	1.49	0.76
1:B:227:VAL:HG21	1:B:233:GLU:HB2	1.66	0.76
1:B:319:MET:SD	1:B:320:GLU:OE1	2.44	0.76
1:A:156:SER:OG	1:A:158:THR:HG22	1.85	0.76
1:A:549:TYR:CE1	1:A:609:ILE:HD11	2.21	0.76
1:C:856:ASN:O	1:C:860:LEU:HB2	1.86	0.76
1:A:875:VAL:HG11	1:A:908:VAL:HG22	1.67	0.75
1:B:588:VAL:HG11	1:C:241:LYS:HD2	1.67	0.75
1:A:888:LEU:HD21	1:A:915:ILE:HG21	1.68	0.75
1:A:816:TRP:O	1:A:820:GLU:HG2	1.86	0.75
1:B:185:THR:O	1:B:185:THR:HG22	1.86	0.75
1:C:319:MET:CE	3:C:1001:BES:HN21	1.98	0.75
1:C:261:THR:HG22	1:C:265:VAL:H	1.50	0.75
1:A:571:THR:HG22	1:A:573:LYS:N	1.98	0.75
1:A:559:THR:HG22	1:A:561:TYR:H	1.50	0.75
1:C:185:THR:O	1:C:185:THR:HG22	1.86	0.74
1:A:185:THR:HG23	1:A:188:ARG:CZ	2.17	0.74
1:B:670:ILE:HD11	1:B:724:GLU:HG3	1.68	0.74
1:C:581:LEU:CD1	1:C:583:LYS:HG3	2.18	0.74
1:B:786:TYR:O	1:B:789:TYR:HB3	1.88	0.73
1:B:908:VAL:O	1:B:908:VAL:HG12	1.87	0.73
1:A:202:SER:OG	1:A:238:VAL:HG12	1.89	0.73
1:C:811:LYS:HE2	1:C:844:VAL:CG1	2.19	0.73
1:B:96:HIS:HD2	1:B:195:ASP:H	1.34	0.73
1:A:183:GLU:HB2	1:A:319:MET:HE1	1.71	0.73
1:C:322:TRP:CE2	1:C:362:ASN:HB3	2.23	0.72
1:A:856:ASN:O	1:A:860:LEU:HB2	1.88	0.72
1:B:571:THR:HG22	1:B:573:LYS:H	1.54	0.72
1:B:113:GLU:O	1:B:117:GLU:CG	2.35	0.72
1:C:68:HIS:CE1	1:C:231:LEU:HD21	2.20	0.72
1:C:908:VAL:O	1:C:908:VAL:HG12	1.88	0.72
1:A:810:ASN:ND2	1:A:813:LYS:HE2	2.04	0.72
1:B:60:PRO:HG3	1:B:194:PHE:CD2	2.25	0.72
1:C:166:THR:HG22	1:C:176:ILE:HD13	1.72	0.72
1:A:581:LEU:CD1	1:A:583:LYS:HG3	2.20	0.71
1:C:640:ILE:CD1	1:C:663:TYR:HE2	1.98	0.71
1:A:319:MET:SD	1:A:320:GLU:OE1	2.48	0.71
1:A:588:VAL:HG12	1:A:589:LEU:N	2.04	0.71
1:C:875:VAL:HG11	1:C:908:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:OE1	1:A:474:LYS:HE3	1.90	0.70
1:B:580:PHE:HZ	1:B:587:ASP:OD2	1.74	0.70
1:B:737:VAL:HG13	1:B:807:ARG:NH2	2.06	0.70
1:B:156:SER:OG	1:B:158:THR:HG22	1.91	0.70
1:C:681:ILE:HB	1:C:682:PRO:HD3	1.73	0.70
1:A:261:THR:HG22	1:A:265:VAL:H	1.56	0.70
1:A:759:GLY:HA3	1:A:788:LYS:HE3	1.74	0.70
1:A:185:THR:HG22	1:A:185:THR:O	1.91	0.70
1:A:67:ILE:HD11	1:A:207:ILE:HD12	1.74	0.70
1:A:571:THR:CG2	1:A:573:LYS:H	2.01	0.69
1:A:888:LEU:HD21	1:A:915:ILE:CG2	2.22	0.69
1:C:185:THR:HG23	1:C:188:ARG:CZ	2.21	0.69
1:A:588:VAL:HG11	1:B:241:LYS:CD	2.21	0.69
1:C:540:ARG:HD2	1:C:591:LEU:O	1.92	0.69
1:B:549:TYR:CD1	1:B:609:ILE:HD11	2.27	0.68
1:C:228:ALA:HB3	1:C:231:LEU:HB2	1.75	0.68
1:A:681:ILE:HB	1:A:682:PRO:HD3	1.74	0.68
1:B:390:THR:HG22	1:B:391:HIS:CD2	2.28	0.68
1:B:399:TYR:OH	1:B:722:VAL:HB	1.92	0.68
1:B:595:VAL:HG12	1:B:597:TRP:H	1.58	0.68
1:C:96:HIS:HD2	1:C:195:ASP:H	1.41	0.68
1:A:570:ILE:HG23	1:A:602:VAL:HG21	1.75	0.68
1:C:533:ILE:HD13	1:C:567:LEU:HD21	1.74	0.68
1:C:319:MET:HE1	3:C:1001:BES:N2	2.05	0.68
1:C:316:SER:N	1:C:317:GLY:HA2	2.08	0.68
1:A:200:LYS:HB2	1:A:241:LYS:HE2	1.75	0.67
1:B:381:PHE:HZ	1:B:449:ARG:HD2	1.58	0.67
1:C:852:PHE:CZ	1:C:856:ASN:ND2	2.61	0.67
1:B:49:TRP:CH2	1:B:51:LYS:HD2	2.29	0.67
1:C:571:THR:HG22	1:C:573:LYS:N	2.10	0.67
1:B:533:ILE:CD1	1:B:567:LEU:HD21	2.25	0.67
1:C:692:MET:SD	1:C:926:PHE:HZ	2.18	0.66
1:C:759:GLY:HA3	1:C:788:LYS:HE3	1.76	0.66
1:B:321:ASN:HB2	1:B:324:LEU:O	1.96	0.66
1:B:763:LEU:CG	1:B:768:THR:HG22	2.24	0.66
1:A:318:ALA:O	3:A:1001:BES:H61	1.95	0.66
1:A:760:ASN:OD1	4:A:6001:NAG:O5	2.13	0.66
1:A:321:ASN:HB2	1:A:324:LEU:O	1.96	0.66
1:A:908:VAL:O	1:A:908:VAL:HG12	1.94	0.66
1:C:546:GLN:HE21	1:C:582:LEU:HD12	1.61	0.66
1:B:464:TYR:OH	1:B:473:THR:HG21	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:VAL:HG12	1:B:589:LEU:N	2.10	0.65
1:B:677:LEU:HD21	1:B:707:LEU:HD11	1.79	0.65
1:B:763:LEU:HD12	1:B:764:PRO:HD2	1.78	0.65
1:B:875:VAL:HG12	1:B:908:VAL:HG11	1.77	0.65
1:A:200:LYS:CE	1:A:365:THR:HG22	2.26	0.65
1:B:559:THR:HG22	1:B:561:TYR:H	1.62	0.65
1:C:671:MET:HB3	1:C:672:PRO:HD3	1.77	0.65
1:A:571:THR:HG23	1:A:595:VAL:HG11	1.78	0.65
1:C:113:GLU:CG	1:C:114:ARG:H	2.05	0.65
1:A:621:THR:HG22	1:A:660:LEU:CG	2.26	0.65
1:A:540:ARG:HD2	1:A:591:LEU:O	1.96	0.65
1:A:763:LEU:CG	1:A:768:THR:HG22	2.27	0.65
1:A:832:PHE:N	1:A:833:PRO:HD2	2.12	0.65
1:B:183:GLU:HB3	1:B:319:MET:HE3	1.78	0.65
1:B:261:THR:HG22	1:B:265:VAL:N	2.07	0.65
1:B:80:THR:HG21	1:B:191:PHE:HB2	1.79	0.64
1:A:390:THR:HG22	1:A:391:HIS:CD2	2.33	0.64
1:A:80:THR:HG21	1:A:191:PHE:HB2	1.80	0.64
1:A:916:GLU:HA	1:A:919:ILE:HD12	1.80	0.64
1:C:121:GLN:HB3	1:C:134:LEU:HB2	1.78	0.64
1:C:156:SER:OG	1:C:158:THR:HG22	1.97	0.64
1:A:139:LEU:HD22	1:A:145:TYR:CE1	2.33	0.64
1:A:81:LYS:HG2	1:A:148:VAL:HG13	1.79	0.64
1:A:883:SER:HB2	1:A:922:MET:HG3	1.80	0.64
1:A:533:ILE:CD1	1:A:567:LEU:HD21	2.27	0.64
1:B:316:SER:N	1:B:317:GLY:HA2	2.11	0.64
1:B:700:LYS:HD3	1:B:738:HIS:HD2	1.62	0.64
1:B:737:VAL:CG1	1:B:807:ARG:HH21	2.06	0.64
1:C:384:PHE:CE2	1:C:400:PHE:HD1	2.15	0.64
1:A:259:LYS:HD3	1:A:287:VAL:HG21	1.80	0.64
1:A:316:SER:N	1:A:317:GLY:HA2	2.11	0.64
1:B:181:GLN:HE22	1:B:319:MET:CE	2.11	0.64
1:B:677:LEU:O	1:B:681:ILE:HG13	1.98	0.64
1:A:700:LYS:HD3	1:A:738:HIS:HD2	1.63	0.64
1:C:764:PRO:O	1:C:768:THR:HG23	1.98	0.63
1:A:108:ARG:HG2	1:A:117:GLU:HG3	1.79	0.63
1:B:167:TYR:CE1	1:B:175:ARG:HB2	2.34	0.63
1:C:581:LEU:HD12	1:C:583:LYS:HG3	1.80	0.63
1:B:832:PHE:N	1:B:833:PRO:HD2	2.13	0.63
1:C:737:VAL:HG11	1:C:807:ARG:NH2	2.13	0.63
1:A:544:MET:HG3	1:A:582:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:HA	1:B:117:GLU:HG3	1.81	0.63
1:C:319:MET:SD	1:C:320:GLU:OE1	2.56	0.63
1:C:837:THR:HG21	1:C:873:HIS:NE2	2.14	0.63
1:B:114:ARG:HA	1:B:117:GLU:CD	2.19	0.63
1:C:97:SER:CB	1:C:131:ILE:HD11	2.28	0.63
1:C:700:LYS:HD3	1:C:738:HIS:CD2	2.34	0.63
1:A:200:LYS:HB3	1:A:241:LYS:HG2	1.81	0.63
1:C:875:VAL:HG12	1:C:908:VAL:HG11	1.81	0.63
1:B:875:VAL:HG11	1:B:908:VAL:HG11	1.78	0.63
1:A:671:MET:HB3	1:A:672:PRO:HD3	1.80	0.62
1:B:261:THR:CG2	1:B:265:VAL:H	2.10	0.62
1:A:96:HIS:CD2	1:A:195:ASP:H	2.15	0.62
1:A:677:LEU:HD21	1:A:707:LEU:HD11	1.81	0.62
1:B:640:ILE:HD11	1:B:676:GLY:HA2	1.81	0.62
1:C:57:TYR:CE1	1:C:90:THR:HG21	2.34	0.62
1:C:700:LYS:HD3	1:C:738:HIS:HD2	1.64	0.62
1:C:75:THR:HG22	1:C:154:ASN:OD1	1.99	0.62
1:B:764:PRO:O	1:B:768:THR:HG23	1.98	0.62
1:B:541:ASN:OD1	1:C:241:LYS:HG3	1.99	0.62
1:C:67:ILE:HD13	1:C:249:PHE:CZ	2.34	0.62
1:A:316:SER:H	1:A:317:GLY:HA2	1.65	0.62
1:C:810:ASN:ND2	1:C:813:LYS:HD3	2.13	0.62
1:A:911:THR:O	1:A:915:ILE:HG13	1.99	0.62
1:A:700:LYS:HD3	1:A:738:HIS:CD2	2.35	0.61
1:B:540:ARG:HD3	1:B:593:GLU:HA	1.82	0.61
1:B:314:PHE:HE2	1:B:316:SER:HB2	1.62	0.61
1:C:68:HIS:HE1	1:C:231:LEU:CD2	2.10	0.61
1:A:117:GLU:O	1:A:118:GLU:HG2	1.99	0.61
1:A:522:ASN:HB3	1:A:526:LEU:HD22	1.82	0.61
1:C:692:MET:SD	1:C:926:PHE:CZ	2.93	0.61
1:A:764:PRO:O	1:A:768:THR:HG23	1.99	0.61
1:B:534:THR:HG21	1:B:613:GLU:OE2	2.00	0.61
1:A:670:ILE:HD13	1:A:727:LEU:HD22	1.82	0.61
1:B:565:VAL:CG1	1:B:582:LEU:HB3	2.30	0.61
1:A:97:SER:CB	1:A:131:ILE:HD11	2.30	0.61
1:A:549:TYR:CD1	1:A:609:ILE:HD11	2.36	0.61
1:B:139:LEU:HD22	1:B:145:TYR:CE1	2.35	0.61
1:B:888:LEU:HD11	1:B:919:ILE:CD1	2.31	0.61
1:A:96:HIS:HD2	1:A:195:ASP:N	1.96	0.61
1:B:543:HIS:CD2	1:B:588:VAL:HG22	2.36	0.61
1:C:318:ALA:O	3:C:1001:BES:H2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG23	1:A:188:ARG:NH2	2.16	0.60
1:A:464:TYR:OH	1:A:473:THR:HG21	2.00	0.60
1:B:261:THR:HG23	1:B:263:SER:N	2.16	0.60
1:A:581:LEU:HD12	1:A:583:LYS:HG3	1.81	0.60
1:A:115:LEU:HD12	1:A:116:SER:H	1.67	0.60
1:C:564:HIS:CD2	1:C:583:LYS:HG2	2.37	0.60
1:C:684:TYR:CD1	1:C:700:LYS:HE2	2.36	0.60
1:C:711:ILE:HD13	1:C:735:ALA:HB2	1.83	0.60
1:B:480:ASP:OD1	1:B:518:LYS:HE2	2.01	0.60
1:C:754:TRP:NE1	1:C:759:GLY:HA2	2.16	0.60
1:A:810:ASN:HD22	1:A:813:LYS:HE2	1.67	0.60
1:B:700:LYS:HD3	1:B:738:HIS:CD2	2.35	0.60
1:C:200:LYS:CE	1:C:365:THR:HG22	2.32	0.60
1:B:757:SER:N	1:B:758:ASN:HA	2.17	0.60
1:A:595:VAL:HG12	1:A:597:TRP:H	1.66	0.60
1:B:114:ARG:HA	1:B:117:GLU:CG	2.32	0.60
1:C:334:PHE:CE1	1:C:338:LYS:HB3	2.37	0.60
1:A:875:VAL:CG2	1:A:908:VAL:HG11	2.31	0.60
1:B:527:GLN:OE1	1:B:563:TRP:NE1	2.34	0.60
1:B:67:ILE:HD13	1:B:249:PHE:CZ	2.36	0.60
1:B:367:GLU:OE1	1:B:474:LYS:HE3	2.01	0.60
1:B:571:THR:HG23	1:B:595:VAL:HG11	1.84	0.60
1:B:757:SER:HB3	1:B:759:GLY:N	2.16	0.59
1:C:183:GLU:HB3	1:C:319:MET:HE3	1.82	0.59
1:A:703:LEU:HD21	1:A:734:LEU:HD21	1.84	0.59
1:B:544:MET:HG3	1:B:582:LEU:CD2	2.27	0.59
1:C:559:THR:CG2	1:C:561:TYR:H	2.15	0.59
1:A:757:SER:N	1:A:758:ASN:HA	2.17	0.59
1:B:316:SER:HB3	3:B:1001:BES:C8	2.31	0.59
1:B:546:GLN:HE21	1:B:582:LEU:HD12	1.67	0.59
1:A:531:PRO:HB3	1:A:563:TRP:CE3	2.38	0.59
1:A:588:VAL:HG12	1:A:589:LEU:H	1.67	0.59
1:C:883:SER:HB2	1:C:922:MET:HG3	1.84	0.59
1:B:363:LEU:HD11	1:B:469:SER:HB2	1.85	0.59
1:B:384:PHE:CE1	1:B:400:PHE:HB2	2.37	0.59
1:B:660:LEU:O	1:B:663:TYR:HD2	1.86	0.59
1:C:832:PHE:N	1:C:833:PRO:HD2	2.18	0.59
1:A:293:TYR:HE2	1:A:382:MET:HG3	1.67	0.59
1:A:660:LEU:O	1:A:663:TYR:HD2	1.85	0.59
1:B:807:ARG:HH12	1:B:843:PRO:HD2	1.68	0.59
1:B:166:THR:HG22	1:B:176:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:VAL:HG12	1:B:582:LEU:HB3	1.85	0.59
1:A:155:LEU:HG	1:A:162:PHE:CE2	2.37	0.58
1:A:741:GLN:HE21	1:A:745:GLN:NE2	2.00	0.58
1:C:754:TRP:CG	1:C:763:LEU:HD11	2.38	0.58
1:A:225:VAL:O	1:A:227:VAL:HG23	2.04	0.58
1:B:741:GLN:HE21	1:B:745:GLN:NE2	2.00	0.58
1:B:115:LEU:HD22	1:B:115:LEU:N	2.18	0.58
1:B:319:MET:SD	1:B:320:GLU:CD	2.81	0.58
1:B:692:MET:SD	1:B:926:PHE:CZ	2.96	0.58
1:A:571:THR:HG23	1:A:595:VAL:CG1	2.34	0.58
1:B:80:THR:HG23	1:B:151:TYR:HE1	1.68	0.58
1:B:313:ASP:O	1:B:315:GLN:HG2	2.04	0.58
1:B:807:ARG:NH1	1:B:843:PRO:HD2	2.19	0.58
1:A:523:THR:O	1:A:527:GLN:HB2	2.03	0.58
1:B:78:GLY:HA3	1:B:151:TYR:CZ	2.38	0.58
1:C:795:SER:OG	1:C:797:GLU:HB3	2.03	0.58
1:A:655:GLU:HB2	1:A:932:TRP:HD1	1.69	0.58
1:B:816:TRP:O	1:B:820:GLU:HG2	2.03	0.58
1:A:261:THR:HG22	1:A:265:VAL:N	2.19	0.58
1:B:237:ASP:OD1	1:B:238:VAL:N	2.37	0.58
1:C:520:MET:SD	1:C:566:PRO:HG3	2.44	0.58
1:B:741:GLN:HE21	1:B:745:GLN:HE21	1.50	0.58
1:C:321:ASN:HB2	1:C:324:LEU:O	2.03	0.58
1:C:588:VAL:HG12	1:C:589:LEU:N	2.19	0.58
1:B:559:THR:CG2	1:B:561:TYR:H	2.17	0.57
1:C:381:PHE:HZ	1:C:449:ARG:HD2	1.69	0.57
1:C:384:PHE:CE1	1:C:400:PHE:HB2	2.39	0.57
1:C:457:PHE:CE2	1:C:461:ILE:HD11	2.39	0.57
1:C:846:TYR:CG	1:C:847:PRO:HD3	2.39	0.57
1:A:643:ALA:O	1:A:647:VAL:HG23	2.05	0.57
1:B:284:ASP:O	1:B:288:THR:HG23	2.04	0.57
1:A:559:THR:CG2	1:A:561:TYR:H	2.16	0.57
1:A:588:VAL:CG1	1:A:589:LEU:N	2.66	0.57
1:B:846:TYR:N	1:B:847:PRO:CD	2.67	0.57
1:C:816:TRP:O	1:C:820:GLU:HG2	2.04	0.57
1:C:89:PRO:O	1:C:90:THR:HG23	2.04	0.57
1:B:451:TYR:HD2	1:B:452:LEU:HD12	1.69	0.57
1:C:850:TRP:O	1:C:854:ARG:HG3	2.05	0.57
1:B:852:PHE:CZ	1:B:856:ASN:ND2	2.72	0.57
1:C:660:LEU:O	1:C:663:TYR:HD2	1.87	0.57
1:C:464:TYR:OH	1:C:473:THR:HG21	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HE1	1:A:231:LEU:HD21	1.70	0.57
1:A:717:THR:OG1	1:A:719:GLU:HG2	2.05	0.57
1:A:786:TYR:O	1:A:789:TYR:HB3	2.05	0.57
1:B:615:ASP:HB2	1:B:618:ASP:HB2	1.85	0.57
1:B:681:ILE:HB	1:B:682:PRO:HD3	1.86	0.57
1:A:261:THR:HG23	1:A:263:SER:H	1.70	0.56
1:A:237:ASP:OD1	1:A:238:VAL:N	2.37	0.56
1:A:588:VAL:CG1	1:A:589:LEU:H	2.17	0.56
1:A:739:ASN:HA	1:A:744:VAL:HG21	1.87	0.56
1:B:523:THR:O	1:B:563:TRP:CD1	2.58	0.56
1:C:733:LEU:O	1:C:737:VAL:HG23	2.05	0.56
1:B:139:LEU:HD22	1:B:145:TYR:HE1	1.70	0.56
1:C:261:THR:HG22	1:C:265:VAL:N	2.19	0.56
1:C:408:MET:HG2	1:C:530:PHE:CE2	2.40	0.56
1:A:327:TYR:HE1	1:A:350:THR:HG22	1.70	0.56
1:B:572:SER:OG	1:B:595:VAL:HG13	2.06	0.56
1:A:200:LYS:HB2	1:A:241:LYS:CE	2.35	0.56
1:A:708:ARG:HG2	1:A:708:ARG:HH11	1.70	0.56
1:B:319:MET:CE	3:B:1001:BES:HN21	2.19	0.56
1:B:810:ASN:CB	1:B:813:LYS:HD2	2.35	0.56
1:A:741:GLN:HE21	1:A:745:GLN:HE21	1.52	0.56
1:A:754:TRP:NE1	1:A:759:GLY:HA2	2.20	0.56
1:B:621:THR:CG2	1:B:660:LEU:HG	2.25	0.56
1:C:156:SER:HB3	1:C:163:TYR:HB3	1.88	0.56
1:C:80:THR:HG21	1:C:191:PHE:HB2	1.86	0.56
1:C:559:THR:HG22	1:C:561:TYR:H	1.71	0.56
1:C:699:PHE:O	1:C:703:LEU:HD13	2.05	0.56
1:B:293:TYR:HE2	1:B:382:MET:HG3	1.70	0.56
1:C:757:SER:N	1:C:758:ASN:HA	2.21	0.56
1:C:757:SER:HB3	1:C:759:GLY:N	2.20	0.56
1:A:272:VAL:HG13	1:A:273:PRO:HD2	1.86	0.56
1:B:281:TYR:CD2	1:B:347:ILE:HD11	2.40	0.56
1:B:876:MET:O	1:B:880:ASN:HB2	2.05	0.56
1:C:281:TYR:CD2	1:C:347:ILE:HD11	2.41	0.56
1:B:913:GLU:O	1:B:916:GLU:HB3	2.06	0.56
1:A:540:ARG:HD3	1:A:593:GLU:HA	1.87	0.55
1:B:791:PHE:H	1:B:791:PHE:HD2	1.54	0.55
1:A:183:GLU:HB2	1:A:319:MET:CE	2.36	0.55
1:A:564:HIS:CD2	1:A:583:LYS:HG2	2.40	0.55
1:A:621:THR:O	1:A:625:LYS:HG3	2.06	0.55
1:B:49:TRP:CZ2	1:B:51:LYS:HD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:LEU:HD22	1:B:801:ILE:HG23	1.88	0.55
1:C:542:VAL:HB	1:C:589:LEU:HB3	1.88	0.55
1:A:681:ILE:HG23	1:A:684:TYR:CZ	2.41	0.55
1:B:281:TYR:HD2	1:B:347:ILE:HD11	1.72	0.55
1:C:230:GLY:C	1:C:231:LEU:HD12	2.26	0.55
1:C:293:TYR:HE2	1:C:382:MET:HG3	1.70	0.55
1:C:383:GLU:O	1:C:387:VAL:HG23	2.06	0.55
1:C:544:MET:HG3	1:C:582:LEU:CD2	2.36	0.55
1:A:853:LEU:O	1:A:857:TRP:HB2	2.06	0.55
1:B:692:MET:SD	1:B:926:PHE:HZ	2.28	0.55
1:C:535:ILE:HG13	1:C:600:PHE:CD1	2.41	0.55
1:A:621:THR:CG2	1:A:660:LEU:HG	2.35	0.55
1:A:837:THR:HG21	1:A:873:HIS:NE2	2.21	0.55
1:B:62:HIS:HE1	1:B:238:VAL:HG13	1.71	0.55
1:C:811:LYS:HE2	1:C:844:VAL:HG13	1.88	0.55
1:C:549:TYR:HE1	1:C:649:ILE:HD13	1.70	0.55
1:B:457:PHE:CD1	1:B:482:MET:HE3	2.42	0.55
1:B:807:ARG:HH12	1:B:843:PRO:CD	2.19	0.55
1:C:97:SER:HB3	1:C:131:ILE:HD11	1.87	0.55
1:C:533:ILE:CD1	1:C:567:LEU:HD21	2.36	0.55
1:B:797:GLU:O	1:B:801:ILE:HG13	2.07	0.55
1:C:699:PHE:CE2	1:C:703:LEU:HD11	2.42	0.55
1:A:757:SER:HB3	1:A:759:GLY:N	2.22	0.55
1:A:927:ASP:O	1:A:931:VAL:HG23	2.07	0.55
1:C:741:GLN:HB3	1:C:742:PRO:HD3	1.89	0.55
1:A:327:TYR:CE1	1:A:350:THR:HG22	2.40	0.54
1:B:185:THR:O	1:B:185:THR:CG2	2.54	0.54
1:C:524:TRP:CZ2	1:C:565:VAL:HG22	2.43	0.54
1:C:846:TYR:CD2	1:C:847:PRO:HD3	2.42	0.54
1:B:911:THR:O	1:B:915:ILE:HG13	2.08	0.54
1:C:803:PHE:O	1:C:807:ARG:HG2	2.07	0.54
1:B:520:MET:SD	1:B:566:PRO:HG3	2.48	0.54
1:B:97:SER:CB	1:B:131:ILE:HD11	2.36	0.54
1:C:219:MET:HE2	1:C:239:THR:HA	1.90	0.54
1:C:546:GLN:HE21	1:C:582:LEU:CD1	2.20	0.54
1:B:812:GLU:O	1:B:816:TRP:HB2	2.08	0.54
1:B:533:ILE:HD12	1:B:567:LEU:HD21	1.89	0.54
1:B:811:LYS:HE2	1:B:844:VAL:CG1	2.38	0.54
1:C:707:LEU:O	1:C:711:ILE:HG13	2.07	0.54
1:A:876:MET:O	1:A:880:ASN:HB2	2.07	0.54
1:B:793:LEU:HG	1:B:794:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ALA:HB2	1:C:332:LEU:HD23	1.90	0.54
1:A:449:ARG:O	1:A:452:LEU:O	2.26	0.54
1:C:390:THR:HG22	1:C:391:HIS:CD2	2.42	0.54
1:A:590:ILE:HG13	1:B:470:TYR:CG	2.42	0.53
1:B:640:ILE:HD11	1:B:676:GLY:CA	2.38	0.53
1:C:803:PHE:CE2	1:C:807:ARG:HG3	2.43	0.53
1:A:167:TYR:CE1	1:A:175:ARG:HB2	2.42	0.53
1:A:806:CYS:SG	1:A:835:ILE:HG23	2.49	0.53
1:A:868:SER:HA	1:A:871:ILE:HG12	1.90	0.53
1:B:588:VAL:CG1	1:B:589:LEU:N	2.71	0.53
1:A:67:ILE:HD11	1:A:207:ILE:CD1	2.37	0.53
1:A:399:TYR:OH	1:A:722:VAL:HB	2.07	0.53
1:B:183:GLU:OE1	1:B:320:GLU:OE2	2.26	0.53
1:B:96:HIS:HD2	1:B:195:ASP:N	2.03	0.53
1:A:76:PHE:HD1	1:A:155:LEU:HD12	1.73	0.53
1:A:185:THR:CG2	1:A:188:ARG:CZ	2.85	0.53
1:C:322:TRP:CE2	1:C:362:ASN:CB	2.91	0.53
1:C:399:TYR:OH	1:C:722:VAL:HB	2.07	0.53
1:A:888:LEU:CD2	1:A:915:ILE:HG21	2.38	0.53
1:B:853:LEU:O	1:B:857:TRP:HB2	2.08	0.53
1:C:444:ILE:HG22	1:C:521:MET:HE1	1.89	0.53
1:B:115:LEU:H	1:B:115:LEU:CD2	2.22	0.53
1:B:115:LEU:CD2	1:B:115:LEU:N	2.71	0.53
1:B:156:SER:HB3	1:B:163:TYR:HB3	1.90	0.53
1:C:611:HIS:CE1	1:C:617:TRP:HE1	2.27	0.53
1:B:580:PHE:CZ	1:B:587:ASP:OD2	2.59	0.53
1:C:185:THR:O	1:C:185:THR:CG2	2.56	0.53
1:C:225:VAL:O	1:C:227:VAL:HG23	2.08	0.53
1:C:571:THR:CG2	1:C:573:LYS:H	2.19	0.53
1:B:181:GLN:HE22	1:B:319:MET:HE3	1.73	0.53
1:B:916:GLU:HA	1:B:919:ILE:HD12	1.90	0.53
1:C:786:TYR:O	1:C:789:TYR:HB3	2.09	0.53
1:A:281:TYR:CD2	1:A:347:ILE:HD11	2.44	0.53
1:A:540:ARG:NH2	1:B:302:PRO:O	2.42	0.53
1:C:139:LEU:HD22	1:C:145:TYR:CE1	2.44	0.53
1:A:763:LEU:HD12	1:A:764:PRO:HD2	1.90	0.52
1:B:96:HIS:CD2	1:B:195:ASP:H	2.20	0.52
1:C:81:LYS:HG2	1:C:148:VAL:HG13	1.91	0.52
1:B:571:THR:HG22	1:B:573:LYS:N	2.22	0.52
1:B:910:GLN:O	1:B:914:THR:HG22	2.09	0.52
1:C:343:SER:O	1:C:347:ILE:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CD1	1:A:203:PHE:CE1	2.97	0.52
1:A:365:THR:O	1:A:472:ASN:HA	2.08	0.52
1:B:167:TYR:CE2	1:B:272:VAL:HG13	2.45	0.52
1:B:582:LEU:CD1	1:B:584:THR:O	2.57	0.52
1:C:888:LEU:HD21	1:C:915:ILE:CG2	2.40	0.52
1:B:230:GLY:C	1:B:231:LEU:HD12	2.30	0.52
1:C:261:THR:HG23	1:C:263:SER:N	2.21	0.52
1:C:621:THR:CG2	1:C:660:LEU:HD13	2.29	0.52
1:C:810:ASN:HD22	1:C:813:LYS:CD	2.20	0.52
1:C:836:LEU:HD22	1:C:874:MET:HE3	1.91	0.52
1:C:449:ARG:O	1:C:452:LEU:O	2.27	0.52
1:C:440:LYS:O	1:C:444:ILE:HG12	2.09	0.52
1:B:185:THR:HG23	1:B:188:ARG:NH2	2.24	0.52
1:C:313:ASP:O	1:C:315:GLN:HG2	2.08	0.52
1:C:717:THR:OG1	1:C:719:GLU:HG2	2.10	0.52
1:A:120:LEU:HD13	1:A:133:LEU:HB3	1.92	0.52
1:B:75:THR:HG22	1:B:154:ASN:OD1	2.10	0.52
1:C:327:TYR:CD2	1:C:332:LEU:HD22	2.45	0.52
1:C:60:PRO:HG3	1:C:194:PHE:CG	2.44	0.52
1:C:117:GLU:O	1:C:118:GLU:HG3	2.08	0.51
1:C:200:LYS:HE3	1:C:365:THR:HG22	1.92	0.51
1:C:214:LEU:HD23	1:C:252:SER:O	2.10	0.51
1:C:684:TYR:HB3	1:C:699:PHE:CD2	2.45	0.51
1:C:286:ALA:O	1:C:290:LEU:HG	2.10	0.51
1:C:259:LYS:HD3	1:C:287:VAL:HG21	1.92	0.51
1:A:582:LEU:CD1	1:A:584:THR:O	2.58	0.51
1:A:405:PHE:CZ	1:A:604:MET:SD	3.03	0.51
1:B:68:HIS:HE1	1:B:231:LEU:HD21	1.75	0.51
1:B:183:GLU:HB3	1:B:319:MET:CE	2.40	0.51
1:B:615:ASP:HB2	1:B:618:ASP:CG	2.31	0.51
1:A:110:GLY:HA3	1:A:114:ARG:O	2.11	0.51
1:A:655:GLU:HB2	1:A:932:TRP:CD1	2.45	0.51
1:B:532:LEU:HD11	1:B:646:LEU:HD21	1.92	0.51
1:C:237:ASP:OD1	1:C:238:VAL:N	2.43	0.51
1:B:888:LEU:HD11	1:B:919:ILE:HD11	1.93	0.51
1:C:571:THR:HG22	1:C:574:SER:H	1.75	0.51
1:C:621:THR:O	1:C:625:LYS:HG3	2.10	0.51
1:A:97:SER:HB2	1:A:131:ILE:HD11	1.91	0.51
1:A:308:LEU:N	1:A:308:LEU:HD12	2.26	0.51
1:C:670:ILE:HD13	1:C:727:LEU:HD22	1.92	0.51
1:A:170:LYS:HG3	1:A:171:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:VAL:HG12	1:A:582:LEU:HB3	1.93	0.51
1:C:322:TRP:CD2	1:C:362:ASN:HB3	2.46	0.51
1:C:595:VAL:HG12	1:C:597:TRP:H	1.76	0.51
1:C:367:GLU:OE1	1:C:474:LYS:HE3	2.10	0.51
1:A:408:MET:HE1	1:A:609:ILE:HG23	1.92	0.50
1:A:533:ILE:HD11	1:A:565:VAL:HG11	1.93	0.50
1:A:761:LEU:HD12	1:A:761:LEU:O	2.10	0.50
1:C:694:GLU:O	1:C:698:GLN:HG3	2.11	0.50
1:A:473:THR:CG2	1:A:474:LYS:N	2.74	0.50
1:A:844:VAL:HG12	1:A:844:VAL:O	2.10	0.50
1:B:536:THR:HB	1:B:543:HIS:HB2	1.93	0.50
1:C:677:LEU:HD21	1:C:707:LEU:HD11	1.92	0.50
1:C:851:GLN:O	1:C:855:LYS:HG3	2.12	0.50
1:B:357:HIS:CE1	1:B:375:ASN:ND2	2.80	0.50
1:B:655:GLU:OE2	1:B:928:LYS:HD3	2.11	0.50
1:C:586:THR:O	1:C:587:ASP:OD1	2.29	0.50
1:A:277:ASN:HD22	1:A:277:ASN:N	2.10	0.50
1:B:181:GLN:HE22	1:B:319:MET:HE2	1.76	0.50
1:B:737:VAL:CG1	1:B:807:ARG:NH2	2.72	0.50
1:C:782:TRP:CD2	1:C:813:LYS:HE3	2.47	0.50
1:C:812:GLU:O	1:C:816:TRP:HB2	2.11	0.50
1:C:876:MET:O	1:C:880:ASN:HB2	2.11	0.50
1:A:573:LYS:HG3	1:A:595:VAL:HG22	1.92	0.50
1:A:757:SER:H	1:A:758:ASN:HA	1.76	0.50
1:A:842:ASN:OD1	1:A:843:PRO:HD2	2.11	0.50
1:C:368:TRP:CG	1:C:369:TRP:N	2.79	0.50
1:C:682:PRO:O	1:C:686:LEU:HD13	2.11	0.50
1:B:185:THR:CG2	1:B:188:ARG:CZ	2.86	0.50
1:B:449:ARG:O	1:B:452:LEU:O	2.30	0.50
1:C:100:LEU:HD22	1:C:151:TYR:HD2	1.77	0.50
1:C:549:TYR:CE1	1:C:609:ILE:HD11	2.46	0.50
1:A:718:ASP:HB3	1:A:725:ARG:NH1	2.26	0.50
1:B:186:ALA:O	1:B:189:MET:HB2	2.11	0.50
1:B:908:VAL:HG12	1:B:911:THR:HB	1.93	0.50
1:C:571:THR:HG23	1:C:595:VAL:CG1	2.41	0.50
1:A:290:LEU:HD12	1:A:359:TRP:HH2	1.77	0.50
1:B:311:ILE:HB	1:B:314:PHE:HB2	1.92	0.50
1:B:523:THR:O	1:B:563:TRP:NE1	2.45	0.50
1:C:737:VAL:CG1	1:C:807:ARG:NH2	2.75	0.50
1:C:907:CYS:C	1:C:909:GLN:H	2.15	0.50
1:A:256:SER:HA	1:A:269:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:MET:CE	1:A:609:ILE:HG23	2.42	0.50
1:C:125:HIS:CD2	1:C:128:GLN:H	2.30	0.50
1:C:884:THR:HG22	1:C:886:THR:H	1.77	0.50
1:C:925:ASN:O	1:C:929:ILE:HG13	2.11	0.50
1:A:588:VAL:CG1	1:B:241:LYS:HD2	2.29	0.49
1:C:571:THR:HG23	1:C:595:VAL:HG11	1.94	0.49
1:A:440:LYS:HE3	1:A:607:TYR:CE2	2.48	0.49
1:A:80:THR:HG23	1:A:151:TYR:CE1	2.36	0.49
1:B:479:TRP:CH2	1:B:521:MET:HE2	2.48	0.49
1:C:314:PHE:CE2	1:C:316:SER:CB	2.84	0.49
1:A:281:TYR:HD2	1:A:347:ILE:HD11	1.76	0.49
1:A:846:TYR:CG	1:A:847:PRO:HD3	2.47	0.49
1:B:875:VAL:HB	1:B:908:VAL:HG21	1.94	0.49
1:C:346:ASP:O	1:C:350:THR:HG23	2.12	0.49
1:A:586:THR:O	1:A:587:ASP:OD1	2.31	0.49
1:B:125:HIS:CD2	1:B:127:ARG:HB3	2.47	0.49
1:C:262:LYS:HG3	1:C:291:GLU:OE2	2.12	0.49
1:C:764:PRO:HB2	1:C:767:VAL:HG22	1.93	0.49
1:C:643:ALA:O	1:C:647:VAL:HG23	2.12	0.49
1:B:366:MET:HG3	1:B:368:TRP:O	2.12	0.49
1:C:183:GLU:HB3	1:C:319:MET:CE	2.42	0.49
1:A:139:LEU:HD22	1:A:145:TYR:HE1	1.75	0.49
1:A:440:LYS:O	1:A:444:ILE:HG12	2.12	0.49
1:A:624:LEU:HD12	1:A:660:LEU:HD21	1.93	0.49
1:A:718:ASP:OD2	1:A:765:VAL:HG22	2.13	0.49
1:A:850:TRP:CE2	1:A:854:ARG:NH1	2.81	0.49
1:A:875:VAL:HG21	1:A:908:VAL:HG11	1.95	0.49
1:B:290:LEU:HD12	1:B:359:TRP:HH2	1.77	0.49
1:B:761:LEU:HD12	1:B:761:LEU:O	2.13	0.49
1:A:177:LEU:HD13	1:A:254:PHE:CZ	2.48	0.49
1:B:107:LEU:HD11	1:B:145:TYR:HB3	1.94	0.49
1:B:210:GLU:HG3	4:B:5001:NAG:H82	1.95	0.49
1:B:785:LEU:CD2	1:B:801:ILE:HG23	2.43	0.49
1:C:348:THR:HG21	1:C:391:HIS:CD2	2.48	0.49
1:C:737:VAL:CG1	1:C:807:ARG:HH21	2.25	0.49
1:A:480:ASP:OD1	1:A:518:LYS:HE2	2.12	0.49
1:A:760:ASN:C	1:A:760:ASN:OD1	2.51	0.49
1:B:844:VAL:O	1:B:844:VAL:HG12	2.13	0.49
1:A:200:LYS:HE2	1:A:365:THR:CG2	2.43	0.48
1:A:908:VAL:HG12	1:A:911:THR:HB	1.95	0.48
1:B:316:SER:CB	3:B:1001:BES:H8	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:THR:HG22	1:B:613:GLU:HG2	1.95	0.48
1:C:908:VAL:CG1	1:C:908:VAL:O	2.60	0.48
1:B:384:PHE:CE2	1:B:400:PHE:HD1	2.32	0.48
1:C:588:VAL:CG1	1:C:589:LEU:N	2.76	0.48
1:A:47:PHE:HA	1:A:48:PRO:HD3	1.61	0.48
1:A:604:MET:HE1	1:A:634:ASN:HB3	1.95	0.48
1:B:225:VAL:O	1:B:227:VAL:HG23	2.13	0.48
1:B:888:LEU:O	1:B:892:LYS:HG3	2.13	0.48
1:C:78:GLY:HA3	1:C:151:TYR:CZ	2.48	0.48
1:B:319:MET:HE2	3:B:1001:BES:C8	2.43	0.48
1:B:214:LEU:HD23	1:B:252:SER:O	2.14	0.48
1:B:533:ILE:HD13	1:B:567:LEU:HD21	1.95	0.48
1:A:536:THR:HB	1:A:543:HIS:HB2	1.95	0.48
1:A:811:LYS:HE2	1:A:844:VAL:CG1	2.43	0.48
1:A:831:GLU:HG2	1:A:835:ILE:HD11	1.95	0.48
1:C:350:THR:HA	3:C:1001:BES:H162	1.95	0.48
1:B:924:LYS:NZ	1:B:924:LYS:HB2	2.29	0.48
1:C:125:HIS:NE2	1:C:128:GLN:HG3	2.29	0.48
1:C:165:SER:O	1:C:177:LEU:HD23	2.14	0.48
1:B:571:THR:HG23	1:B:595:VAL:CG1	2.43	0.48
1:B:815:GLN:HA	1:B:818:LEU:HD12	1.96	0.48
1:B:908:VAL:HG13	1:B:911:THR:OG1	2.14	0.48
1:C:139:LEU:HD22	1:C:145:TYR:HE1	1.78	0.48
1:A:669:GLU:O	1:A:672:PRO:HD2	2.14	0.48
1:B:319:MET:HE1	3:B:1001:BES:HN21	1.78	0.48
1:B:292:PHE:CZ	1:B:386:SER:HA	2.49	0.48
1:B:378:PHE:CE1	1:B:461:ILE:HD13	2.48	0.48
1:C:325:THR:HG23	1:C:327:TYR:CE2	2.48	0.48
1:C:544:MET:CG	1:C:582:LEU:HD23	2.43	0.48
1:C:846:TYR:N	1:C:847:PRO:CD	2.76	0.48
1:A:210:GLU:HG3	4:A:5001:NAG:H82	1.86	0.48
1:A:67:ILE:O	1:A:67:ILE:HG13	2.13	0.48
1:C:444:ILE:CG2	1:C:521:MET:HE1	2.43	0.48
1:C:754:TRP:CE2	1:C:759:GLY:HA2	2.49	0.48
1:A:444:ILE:HG22	1:A:521:MET:HE1	1.96	0.48
1:A:821:SER:HA	1:A:827:ILE:HG23	1.96	0.48
1:B:367:GLU:OE1	1:B:474:LYS:CE	2.62	0.48
1:B:62:HIS:ND1	1:B:202:SER:HB2	2.29	0.48
1:B:457:PHE:CD1	1:B:482:MET:CE	2.97	0.47
1:B:615:ASP:HB2	1:B:618:ASP:CB	2.44	0.47
1:B:682:PRO:O	1:B:686:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:CD2	1:C:355:LEU:HD13	2.44	0.47
1:A:565:VAL:CG1	1:A:582:LEU:HB3	2.44	0.47
1:B:846:TYR:CD2	1:B:847:PRO:HD3	2.49	0.47
1:B:316:SER:H	1:B:317:GLY:HA2	1.77	0.47
1:B:49:TRP:CZ2	1:B:51:LYS:HB2	2.49	0.47
1:B:782:TRP:HZ2	1:B:817:LEU:HD11	1.79	0.47
1:B:701:ALA:O	1:B:705:ARG:HG3	2.14	0.47
1:B:704:ILE:O	1:B:708:ARG:HB2	2.15	0.47
1:B:588:VAL:CG1	1:C:241:LYS:HD2	2.39	0.47
1:A:740:TYR:O	1:A:744:VAL:HG23	2.14	0.47
1:B:837:THR:HG21	1:B:873:HIS:NE2	2.29	0.47
1:C:916:GLU:HA	1:C:919:ILE:HD12	1.96	0.47
1:A:202:SER:OG	1:A:238:VAL:CG1	2.61	0.47
1:B:582:LEU:HD11	1:B:584:THR:O	2.13	0.47
1:C:544:MET:SD	1:C:580:PHE:CE2	3.07	0.47
1:A:569:PHE:CZ	1:A:589:LEU:HD21	2.50	0.47
1:A:826:LYS:O	1:A:827:ILE:HB	2.15	0.47
1:A:846:TYR:N	1:A:847:PRO:CD	2.77	0.47
1:B:588:VAL:CG1	1:B:589:LEU:H	2.28	0.47
1:C:371:ASP:OD1	1:C:475:ASN:ND2	2.48	0.47
1:A:115:LEU:HD12	1:A:116:SER:N	2.29	0.47
1:A:229:GLU:HA	1:A:229:GLU:OE1	2.15	0.47
1:A:257:VAL:HG23	1:A:283:LEU:HD22	1.96	0.47
1:C:405:PHE:CZ	1:C:604:MET:SD	3.08	0.47
1:C:613:GLU:HG3	1:C:614:ASP:N	2.29	0.47
1:C:853:LEU:O	1:C:857:TRP:HB2	2.15	0.47
1:B:532:LEU:HD12	1:B:609:ILE:O	2.15	0.47
1:A:159:PHE:CE1	1:A:313:ASP:HB3	2.49	0.47
1:A:246:LEU:CD2	1:A:320:GLU:HG2	2.45	0.47
1:B:200:LYS:CE	1:B:365:THR:HG22	2.45	0.47
1:C:53:ARG:HD3	1:C:368:TRP:CH2	2.50	0.47
1:C:624:LEU:O	1:C:628:HIS:HB3	2.15	0.47
1:B:272:VAL:HG13	1:B:273:PRO:HD2	1.97	0.47
1:B:570:ILE:HG23	1:B:602:VAL:HG21	1.95	0.47
1:A:160:HIS:CD2	1:A:186:ALA:HB2	2.50	0.46
1:C:100:LEU:HD22	1:C:151:TYR:CD2	2.50	0.46
1:C:710:LEU:CD2	1:C:731:LEU:HD11	2.45	0.46
1:A:692:MET:SD	1:A:926:PHE:CZ	3.08	0.46
1:C:334:PHE:HE1	1:C:338:LYS:HB3	1.79	0.46
1:A:582:LEU:HD11	1:A:584:THR:O	2.14	0.46
1:A:63:TYR:HB2	1:A:203:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:VAL:HG21	1:C:233:GLU:CB	2.33	0.46
1:C:733:LEU:HA	1:C:770:ALA:HB2	1.98	0.46
1:C:888:LEU:HD11	1:C:919:ILE:CD1	2.44	0.46
1:A:384:PHE:CE2	1:A:400:PHE:HD1	2.34	0.46
1:B:314:PHE:HE2	1:B:317:GLY:C	2.19	0.46
1:C:133:LEU:HD13	1:C:147:VAL:HG11	1.97	0.46
1:C:181:GLN:OE1	1:C:319:MET:HE3	2.15	0.46
1:C:757:SER:H	1:C:758:ASN:HA	1.81	0.46
1:A:200:LYS:HE2	1:A:365:THR:HG22	1.98	0.46
1:A:565:VAL:HA	1:A:566:PRO:HD3	1.68	0.46
1:B:297:PHE:O	1:B:299:ILE:HG13	2.15	0.46
1:A:156:SER:HG	1:A:158:THR:HG22	1.81	0.46
1:A:852:PHE:CZ	1:A:856:ASN:ND2	2.79	0.46
1:B:763:LEU:CD2	1:B:768:THR:HG22	2.45	0.46
1:C:281:TYR:HD2	1:C:347:ILE:HD11	1.80	0.46
1:C:544:MET:HG3	1:C:582:LEU:HD21	1.98	0.46
1:C:806:CYS:SG	1:C:835:ILE:HG23	2.55	0.46
1:A:858:ASN:O	1:A:861:VAL:HG22	2.16	0.46
1:C:615:ASP:HB3	1:C:618:ASP:HB2	1.98	0.46
1:C:761:LEU:O	1:C:761:LEU:HD12	2.16	0.46
1:C:844:VAL:O	1:C:844:VAL:HG12	2.16	0.46
1:C:89:PRO:O	1:C:90:THR:CG2	2.64	0.46
1:B:925:ASN:O	1:B:929:ILE:HG13	2.15	0.46
1:B:702:PHE:CZ	1:B:932:TRP:CH2	3.04	0.46
1:A:268:SER:HB2	1:A:307:ASP:OD1	2.16	0.46
1:A:641:ASN:O	1:A:645:GLN:HG3	2.15	0.46
1:B:846:TYR:CG	1:B:847:PRO:HD3	2.51	0.46
1:B:654:ILE:HB	1:B:925:ASN:ND2	2.30	0.46
1:C:196:GLU:HB2	1:C:199:PHE:HD2	1.80	0.46
1:C:384:PHE:HE1	1:C:396:VAL:O	1.99	0.46
1:C:580:PHE:CD1	1:C:589:LEU:HD13	2.51	0.46
1:C:913:GLU:O	1:C:916:GLU:HB3	2.16	0.46
1:A:269:VAL:HG11	1:A:279:ALA:HB1	1.98	0.45
1:A:875:VAL:HG22	1:A:908:VAL:HG11	1.97	0.45
1:B:868:SER:HA	1:B:871:ILE:HG12	1.97	0.45
1:B:590:ILE:HG13	1:C:470:TYR:CG	2.52	0.45
1:A:156:SER:HB3	1:A:163:TYR:HB3	1.97	0.45
1:C:411:ASP:OD1	1:C:529:GLY:HA2	2.15	0.45
1:C:879:THR:OG1	1:C:911:THR:HG21	2.16	0.45
1:C:827:ILE:HD11	1:C:830:GLN:HE21	1.81	0.45
1:A:261:THR:HG23	1:A:263:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ILE:HG23	1:A:684:TYR:OH	2.17	0.45
1:C:319:MET:SD	1:C:320:GLU:CD	2.94	0.45
1:A:888:LEU:O	1:A:892:LYS:HG3	2.16	0.45
1:B:227:VAL:HG21	1:B:233:GLU:CB	2.42	0.45
1:B:876:MET:HG2	1:B:911:THR:OG1	2.17	0.45
1:A:331:ALA:HA	1:A:347:ILE:HG22	1.99	0.45
1:A:613:GLU:HG3	1:A:614:ASP:N	2.31	0.45
1:A:640:ILE:HD11	1:A:663:TYR:CE2	2.52	0.45
1:A:694:GLU:HG2	1:A:695:VAL:N	2.30	0.45
1:B:181:GLN:NE2	3:B:1001:BES:C9	2.80	0.45
1:B:875:VAL:CB	1:B:908:VAL:HG21	2.47	0.45
1:C:684:TYR:HA	1:C:687:MET:SD	2.57	0.45
1:A:434:ASP:OD1	1:A:435:ASP:N	2.48	0.45
1:A:548:HIS:HB2	1:A:561:TYR:HB2	1.98	0.45
1:A:848:LEU:O	1:A:852:PHE:HB2	2.17	0.45
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.79	0.45
1:B:65:LEU:HD23	1:B:80:THR:HB	1.99	0.45
1:B:757:SER:H	1:B:758:ASN:HA	1.82	0.45
1:C:177:LEU:HD13	1:C:254:PHE:CZ	2.52	0.45
1:C:667:GLU:HG2	1:C:672:PRO:HB2	1.99	0.45
1:C:655:GLU:HB3	1:C:932:TRP:CD1	2.52	0.45
1:A:62:HIS:ND1	1:A:202:SER:HB3	2.31	0.45
1:B:548:HIS:ND1	1:B:559:THR:HG21	2.32	0.45
1:C:378:PHE:CZ	1:C:382:MET:HE2	2.52	0.45
1:C:582:LEU:HD11	1:C:584:THR:O	2.17	0.45
1:B:687:MET:SD	1:B:695:VAL:HG12	2.57	0.45
1:C:227:VAL:CG2	1:C:233:GLU:HB2	2.34	0.45
1:B:156:SER:HB3	1:B:163:TYR:CB	2.47	0.44
1:A:846:TYR:CD2	1:A:847:PRO:HD3	2.53	0.44
1:A:868:SER:HA	1:A:871:ILE:CD1	2.48	0.44
1:B:718:ASP:HB3	1:B:725:ARG:NH1	2.32	0.44
1:C:384:PHE:O	1:C:385:VAL:C	2.54	0.44
1:C:604:MET:HG2	1:C:604:MET:O	2.17	0.44
1:A:131:ILE:HG22	1:A:132:ALA:N	2.32	0.44
1:C:405:PHE:HZ	1:C:604:MET:SD	2.40	0.44
1:C:647:VAL:HA	1:C:652:LEU:O	2.17	0.44
1:C:852:PHE:CE1	1:C:856:ASN:ND2	2.85	0.44
1:A:215:ALA:HA	1:A:250:ILE:O	2.18	0.44
1:A:763:LEU:CD2	1:A:768:THR:HG22	2.46	0.44
1:B:301:TYR:HA	1:B:302:PRO:HD3	1.80	0.44
1:C:457:PHE:CD1	1:C:482:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:PHE:HA	1:C:48:PRO:HD3	1.62	0.44
1:C:65:LEU:HD22	1:C:80:THR:CG2	2.48	0.44
1:A:185:THR:CG2	1:A:185:THR:O	2.63	0.44
1:A:49:TRP:CZ3	1:A:55:PRO:HG3	2.52	0.44
1:B:185:THR:HG23	1:B:188:ARG:NE	2.33	0.44
1:B:411:ASP:OD1	1:B:529:GLY:N	2.51	0.44
1:C:876:MET:HG2	1:C:911:THR:OG1	2.18	0.44
1:C:183:GLU:OE1	1:C:320:GLU:OE2	2.35	0.44
1:B:256:SER:HA	1:B:269:VAL:O	2.17	0.44
1:B:56:GLU:H	1:B:56:GLU:HG2	1.63	0.44
1:B:595:VAL:HG12	1:B:597:TRP:N	2.29	0.44
1:A:324:LEU:HG	1:A:324:LEU:O	2.18	0.44
1:A:879:THR:OG1	1:A:911:THR:HG21	2.17	0.44
1:B:74:LEU:HD13	1:B:164:LYS:HD3	2.00	0.44
1:A:613:GLU:HG3	1:A:614:ASP:H	1.83	0.44
1:A:682:PRO:O	1:A:686:LEU:HD13	2.17	0.44
1:B:791:PHE:N	1:B:791:PHE:CD2	2.86	0.44
1:C:436:VAL:O	1:C:439:ASP:HB2	2.17	0.44
1:A:97:SER:HB3	1:A:131:ILE:CG1	2.48	0.43
1:A:139:LEU:HB3	1:A:145:TYR:CE1	2.53	0.43
1:A:227:VAL:CG2	1:A:233:GLU:HB2	2.38	0.43
1:B:534:THR:CG2	1:B:613:GLU:HG2	2.49	0.43
1:B:670:ILE:HD11	1:B:724:GLU:HA	2.00	0.43
1:C:277:ASN:HD22	1:C:277:ASN:N	2.16	0.43
1:C:537:VAL:HG22	1:C:542:VAL:HG22	1.99	0.43
1:C:797:GLU:O	1:C:801:ILE:HG13	2.18	0.43
1:A:556:ALA:HB3	1:A:557:PRO:HD3	1.99	0.43
1:B:160:HIS:CD2	1:B:186:ALA:HB2	2.54	0.43
1:B:196:GLU:HB2	1:B:199:PHE:HD2	1.84	0.43
1:C:367:GLU:OE1	1:C:474:LYS:CE	2.66	0.43
1:C:384:PHE:CE2	1:C:400:PHE:CD1	3.03	0.43
1:C:565:VAL:HA	1:C:566:PRO:HD3	1.71	0.43
1:C:754:TRP:HA	1:C:757:SER:HB2	2.00	0.43
1:A:708:ARG:HG2	1:A:708:ARG:NH1	2.34	0.43
1:C:125:HIS:CE1	1:C:128:GLN:NE2	2.87	0.43
1:C:457:PHE:CE2	1:C:461:ILE:CD1	3.01	0.43
1:C:68:HIS:CE1	1:C:231:LEU:CD2	2.94	0.43
1:A:314:PHE:HE2	1:A:316:SER:HB2	1.77	0.43
1:A:604:MET:HG2	1:A:604:MET:O	2.17	0.43
1:A:907:CYS:C	1:A:909:GLN:H	2.22	0.43
1:B:444:ILE:HG22	1:B:521:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:ASN:HA	1:B:744:VAL:HG21	2.00	0.43
1:C:345:LEU:HD11	1:C:396:VAL:HG12	2.01	0.43
1:C:457:PHE:CD1	1:C:482:MET:CE	3.01	0.43
1:C:544:MET:SD	1:C:567:LEU:HD12	2.59	0.43
1:C:94:ILE:HD12	1:C:94:ILE:N	2.33	0.43
1:B:434:ASP:HB3	1:B:435:ASP:H	1.70	0.43
1:C:858:ASN:O	1:C:861:VAL:HG22	2.19	0.43
1:A:214:LEU:HD23	1:A:252:SER:O	2.18	0.43
1:A:219:MET:HG2	1:A:239:THR:HG22	2.01	0.43
1:A:368:TRP:CG	1:A:369:TRP:N	2.87	0.43
1:B:405:PHE:CZ	1:B:604:MET:SD	3.12	0.43
1:B:611:HIS:ND1	1:B:646:LEU:HD13	2.32	0.43
1:B:879:THR:OG1	1:B:911:THR:HG21	2.18	0.43
1:C:160:HIS:CD2	1:C:186:ALA:HB2	2.54	0.43
1:C:373:TRP:HA	1:C:438:TYR:CE2	2.53	0.43
1:C:544:MET:SD	1:C:580:PHE:CD2	3.12	0.43
1:B:378:PHE:HE1	1:B:461:ILE:HD13	1.82	0.43
1:B:684:TYR:C	1:B:684:TYR:CD1	2.92	0.43
1:B:793:LEU:O	1:B:794:SER:HB2	2.19	0.43
1:C:159:PHE:CE1	1:C:313:ASP:HB3	2.54	0.43
1:C:185:THR:CG2	1:C:188:ARG:CZ	2.95	0.43
1:C:380:LYS:HE3	1:C:435:ASP:OD1	2.18	0.43
1:C:572:SER:OG	1:C:595:VAL:HG13	2.18	0.43
1:C:701:ALA:O	1:C:705:ARG:HG3	2.18	0.43
1:C:868:SER:HA	1:C:871:ILE:HG12	1.99	0.43
1:A:568:THR:HA	1:A:578:HIS:O	2.19	0.43
1:B:118:GLU:HA	1:B:119:PRO:HD3	1.92	0.43
1:B:449:ARG:O	1:B:449:ARG:HG2	2.19	0.43
1:B:888:LEU:HD21	1:B:915:ILE:CG2	2.49	0.43
1:C:810:ASN:CB	1:C:813:LYS:HD3	2.49	0.43
1:A:457:PHE:CD1	1:A:482:MET:HE3	2.54	0.43
1:B:115:LEU:HD13	1:B:115:LEU:HA	1.79	0.43
1:A:78:GLY:HA3	1:A:151:TYR:CZ	2.54	0.42
1:A:590:ILE:HG13	1:B:470:TYR:CD1	2.53	0.42
1:B:792:SER:OG	1:B:793:LEU:N	2.51	0.42
1:C:620:LEU:HD13	1:C:639:LEU:HD21	2.01	0.42
1:C:741:GLN:HE21	1:C:745:GLN:NE2	2.17	0.42
1:C:782:TRP:CE2	1:C:805:LEU:HD22	2.54	0.42
1:A:293:TYR:CE2	1:A:382:MET:HG3	2.52	0.42
1:A:810:ASN:ND2	1:A:813:LYS:HG3	2.34	0.42
1:A:815:GLN:HA	1:A:818:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD13	1:B:254:PHE:CZ	2.54	0.42
1:B:328:ARG:CZ	1:B:331:ALA:HB2	2.49	0.42
1:B:782:TRP:CE2	1:B:805:LEU:HD22	2.54	0.42
1:B:888:LEU:HD21	1:B:915:ILE:HG22	2.01	0.42
1:C:373:TRP:HA	1:C:438:TYR:CD2	2.54	0.42
1:C:850:TRP:CE3	1:C:850:TRP:HA	2.54	0.42
1:A:261:THR:CG2	1:A:265:VAL:H	2.29	0.42
1:A:411:ASP:CG	1:A:529:GLY:HA2	2.39	0.42
1:B:408:MET:CE	1:B:609:ILE:HG23	2.49	0.42
1:C:269:VAL:HG11	1:C:279:ALA:HB1	2.01	0.42
1:C:480:ASP:OD1	1:C:518:LYS:HE2	2.19	0.42
1:C:543:HIS:NE2	1:C:586:THR:OG1	2.42	0.42
1:A:569:PHE:CD1	1:A:598:ILE:HD11	2.55	0.42
1:A:681:ILE:HD13	1:A:684:TYR:OH	2.20	0.42
1:A:885:ARG:O	1:A:888:LEU:HB2	2.20	0.42
1:B:702:PHE:CE1	1:B:932:TRP:CZ3	3.08	0.42
1:C:107:LEU:HB2	1:C:120:LEU:HD21	2.01	0.42
1:A:311:ILE:HB	1:A:314:PHE:HB2	2.00	0.42
1:A:343:SER:O	1:A:347:ILE:HG23	2.19	0.42
1:A:473:THR:HG22	1:A:474:LYS:N	2.33	0.42
1:A:595:VAL:HG12	1:A:596:GLU:N	2.34	0.42
1:B:702:PHE:CE1	1:B:932:TRP:HZ3	2.38	0.42
1:C:128:GLN:O	1:C:130:GLN:HG3	2.20	0.42
4:C:5002:NAG:O7	6:C:5005:MAN:H62	2.20	0.42
1:A:183:GLU:HA	1:A:184:PRO:HA	1.82	0.42
1:A:621:THR:HG22	1:A:660:LEU:CD2	2.49	0.42
1:B:314:PHE:CE2	1:B:317:GLY:C	2.93	0.42
1:C:556:ALA:N	1:C:557:PRO:CD	2.82	0.42
1:C:732:LEU:CD1	1:C:767:VAL:HG12	2.49	0.42
1:C:888:LEU:O	1:C:892:LYS:HG3	2.20	0.42
1:A:125:HIS:CE1	1:A:128:GLN:NE2	2.88	0.42
1:A:207:ILE:HG12	1:A:236:PHE:HE1	1.85	0.42
1:A:457:PHE:CD1	1:A:482:MET:CE	3.03	0.42
1:A:520:MET:HA	1:A:564:HIS:HB2	2.01	0.42
1:B:384:PHE:O	1:B:385:VAL:C	2.57	0.42
1:B:556:ALA:N	1:B:557:PRO:CD	2.82	0.42
1:C:125:HIS:HD2	1:C:128:GLN:H	1.66	0.42
1:C:473:THR:CG2	1:C:474:LYS:N	2.82	0.42
1:C:613:GLU:HG3	1:C:614:ASP:H	1.85	0.42
1:A:367:GLU:OE1	1:A:474:LYS:CE	2.63	0.42
1:A:366:MET:HG3	1:A:368:TRP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:ALA:O	1:A:875:VAL:CG1	2.61	0.42
1:B:90:THR:O	1:B:139:LEU:HG	2.20	0.42
1:B:599:LYS:HE2	1:B:639:LEU:HG	2.00	0.42
1:C:464:TYR:CE1	1:C:473:THR:HG21	2.55	0.42
1:C:850:TRP:HE3	1:C:850:TRP:HA	1.84	0.42
1:A:379:ALA:O	1:A:383:GLU:HG3	2.20	0.42
1:A:702:PHE:CZ	1:A:932:TRP:CH2	3.08	0.42
1:B:181:GLN:NE2	3:B:1001:BES:H9	2.35	0.42
1:B:835:ILE:O	1:B:839:ILE:HG13	2.20	0.42
1:C:924:LYS:HD3	1:C:924:LYS:O	2.20	0.42
1:A:168:ARG:HA	1:A:173:GLU:O	2.20	0.42
1:A:850:TRP:HE3	1:A:850:TRP:HA	1.85	0.42
1:C:378:PHE:CZ	1:C:382:MET:CE	3.03	0.42
1:A:245:TYR:HE2	1:A:320:GLU:OE2	2.03	0.41
1:A:67:ILE:HD13	1:A:249:PHE:CE1	2.55	0.41
1:A:314:PHE:HE2	1:A:317:GLY:C	2.24	0.41
1:A:544:MET:HE2	1:A:567:LEU:CD1	2.50	0.41
1:A:792:SER:O	1:A:793:LEU:HB2	2.20	0.41
1:B:562:LEU:HD22	1:B:562:LEU:HA	1.92	0.41
1:C:366:MET:HG3	1:C:368:TRP:O	2.20	0.41
1:C:478:LEU:HD13	1:C:479:TRP:CZ3	2.55	0.41
1:C:698:GLN:HE21	1:C:698:GLN:HB3	1.70	0.41
1:A:186:ALA:O	1:A:189:MET:HB2	2.19	0.41
1:A:411:ASP:OD1	1:A:529:GLY:N	2.51	0.41
1:A:603:GLY:O	1:A:604:MET:HB3	2.20	0.41
1:A:752:ARG:HB2	1:A:752:ARG:HE	1.60	0.41
1:B:440:LYS:O	1:B:444:ILE:HG12	2.20	0.41
1:B:520:MET:HG3	1:B:564:HIS:HB2	2.03	0.41
1:C:411:ASP:OD1	1:C:529:GLY:N	2.53	0.41
1:C:754:TRP:CD1	1:C:763:LEU:HD11	2.55	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.90	0.41
1:A:842:ASN:HA	1:A:843:PRO:HD2	1.92	0.41
1:B:100:LEU:HD22	1:B:151:TYR:CD2	2.56	0.41
1:B:390:THR:CG2	1:B:391:HIS:CD2	3.02	0.41
1:B:733:LEU:O	1:B:737:VAL:HG23	2.19	0.41
1:C:322:TRP:CZ2	1:C:363:LEU:HA	2.56	0.41
1:A:67:ILE:CD1	1:A:249:PHE:CE1	3.03	0.41
1:A:229:GLU:OE1	6:A:5004:MAN:O2	2.39	0.41
1:A:807:ARG:NH1	1:A:843:PRO:HD2	2.35	0.41
1:B:97:SER:HB3	1:B:131:ILE:HD11	2.01	0.41
1:B:183:GLU:HA	1:B:184:PRO:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:TRP:CE3	1:B:850:TRP:HA	2.56	0.41
1:C:185:THR:HG23	1:C:188:ARG:NH2	2.35	0.41
1:A:807:ARG:HH12	1:A:843:PRO:HD2	1.84	0.41
1:A:884:THR:HG22	1:A:886:THR:H	1.86	0.41
1:B:97:SER:HB3	1:B:131:ILE:CG1	2.51	0.41
1:C:544:MET:HG3	1:C:582:LEU:HD23	2.01	0.41
1:C:755:LYS:C	1:C:757:SER:H	2.24	0.41
1:A:242:MET:HB3	1:A:322:TRP:CZ3	2.55	0.41
1:A:764:PRO:O	1:A:767:VAL:HG22	2.20	0.41
1:A:884:THR:HB	1:A:887:ARG:HB2	2.02	0.41
1:B:228:ALA:HB3	1:B:231:LEU:HB2	2.02	0.41
1:B:451:TYR:CD2	1:B:452:LEU:HD12	2.51	0.41
1:B:850:TRP:HE3	1:B:850:TRP:HA	1.85	0.41
1:A:155:LEU:HG	1:A:162:PHE:CD2	2.56	0.41
1:A:200:LYS:CB	1:A:241:LYS:HG2	2.49	0.41
1:A:342:SER:O	1:A:346:ASP:N	2.44	0.41
1:A:378:PHE:CE1	1:A:461:ILE:HD13	2.55	0.41
1:B:277:ASN:ND2	1:B:278:GLN:HG3	2.36	0.41
1:B:368:TRP:CG	1:B:369:TRP:N	2.89	0.41
1:B:520:MET:HG3	1:B:564:HIS:CB	2.51	0.41
1:B:624:LEU:HD12	1:B:660:LEU:HD21	2.03	0.41
1:B:699:PHE:HE2	1:B:703:LEU:HD11	1.86	0.41
1:B:810:ASN:HB2	1:B:813:LYS:HD2	2.03	0.41
1:C:183:GLU:HA	1:C:184:PRO:HA	1.85	0.41
1:C:328:ARG:CZ	1:C:331:ALA:HB2	2.51	0.41
1:C:731:LEU:HD23	1:C:731:LEU:HA	1.75	0.41
1:A:320:GLU:OE1	1:A:320:GLU:N	2.46	0.41
1:B:851:GLN:O	1:B:855:LYS:HG3	2.20	0.41
1:A:162:PHE:CD1	1:A:249:PHE:HE1	2.39	0.41
1:A:319:MET:HE1	1:A:320:GLU:OE2	2.21	0.41
1:A:850:TRP:CE3	1:A:850:TRP:HA	2.55	0.41
1:B:406:ASP:O	1:B:410:VAL:HG23	2.21	0.41
1:C:739:ASN:HA	1:C:744:VAL:HG21	2.02	0.41
1:A:62:HIS:HE1	1:A:238:VAL:HG13	1.86	0.41
1:A:301:TYR:HA	1:A:302:PRO:HD3	1.86	0.41
1:B:681:ILE:N	1:B:682:PRO:CD	2.84	0.41
1:B:764:PRO:HB2	1:B:767:VAL:HG22	2.02	0.41
1:C:548:HIS:ND1	1:C:559:THR:HG21	2.36	0.41
1:A:556:ALA:N	1:A:557:PRO:CD	2.84	0.40
1:B:331:ALA:HA	1:B:347:ILE:HG22	2.03	0.40
1:B:533:ILE:HD11	1:B:565:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:ASN:CG	1:B:813:LYS:HD2	2.42	0.40
1:B:815:GLN:O	1:B:818:LEU:HB2	2.20	0.40
1:C:908:VAL:HG13	1:C:911:THR:OG1	2.21	0.40
1:A:177:LEU:HD13	1:A:254:PHE:HZ	1.86	0.40
1:A:310:ALA:HB2	1:A:332:LEU:HD23	2.03	0.40
1:A:758:ASN:C	1:A:760:ASN:N	2.73	0.40
1:B:556:ALA:HB3	1:B:557:PRO:HD3	2.02	0.40
1:C:125:HIS:CD2	1:C:128:GLN:HG3	2.57	0.40
1:C:337:GLU:HG3	1:C:337:GLU:O	2.21	0.40
1:C:710:LEU:HG	1:C:731:LEU:CD1	2.51	0.40
1:C:827:ILE:CD1	1:C:830:GLN:HE21	2.34	0.40
1:B:114:ARG:CA	1:B:117:GLU:HG3	2.49	0.40
1:B:603:GLY:O	1:B:604:MET:HB3	2.20	0.40
1:C:96:HIS:CD2	1:C:195:ASP:HB3	2.56	0.40
1:C:357:HIS:CE1	1:C:375:ASN:ND2	2.89	0.40
1:A:139:LEU:HB3	1:A:145:TYR:HE1	1.87	0.40
1:A:196:GLU:HB2	1:A:199:PHE:HD2	1.86	0.40
1:A:449:ARG:HG3	1:A:457:PHE:CG	2.56	0.40
1:A:595:VAL:HG12	1:A:597:TRP:N	2.36	0.40
1:B:277:ASN:HD22	1:B:277:ASN:N	2.19	0.40
1:C:183:GLU:OE1	3:C:1001:BES:N2	2.55	0.40
1:C:167:TYR:CE1	1:C:175:ARG:HB2	2.57	0.40
1:C:261:THR:CG2	1:C:265:VAL:HB	2.51	0.40
1:C:911:THR:O	1:C:915:ILE:HG13	2.21	0.40
1:A:707:LEU:O	1:A:708:ARG:C	2.59	0.40
1:A:837:THR:O	1:A:841:ARG: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	804/921 (87%)	750 (93%)	50 (6%)	4 (0%)	32	71
1	B	809/921 (88%)	755 (93%)	52 (6%)	2 (0%)	51	84
1	C	805/921 (87%)	753 (94%)	51 (6%)	1 (0%)	55	87
All	All	2418/2763 (88%)	2258 (93%)	153 (6%)	7 (0%)	44	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	908	VAL
1	A	229	GLU
1	A	908	VAL
1	B	908	VAL
1	A	855	LYS
1	B	855	LYS
1	A	827	ILE

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	733/819 (90%)	710 (97%)	23 (3%)	45	78
1	B	734/819 (90%)	711 (97%)	23 (3%)	45	78
1	C	734/819 (90%)	711 (97%)	23 (3%)	45	78
All	All	2201/2457 (90%)	2132 (97%)	69 (3%)	45	78

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	114	ARG
1	A	174	LEU
1	A	175	ARG
1	A	177	LEU
1	A	209	ARG

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Mol	Chain	Res	Type
1	A	277	ASN
1	A	303	LEU
1	A	305	LYS
1	A	322	TRP
1	A	366	MET
1	A	395	LYS
1	A	526	LEU
1	A	544	MET
1	A	660	LEU
1	A	743	CYS
1	A	779	THR
1	A	850	TRP
1	A	853	LEU
1	A	885	ARG
1	A	886	THR
1	A	924	LYS
1	A	934	GLN
1	B	95	LEU
1	B	174	LEU
1	B	175	ARG
1	B	177	LEU
1	B	209	ARG
1	B	277	ASN
1	B	303	LEU
1	B	305	LYS
1	B	322	TRP
1	B	366	MET
1	B	544	MET
1	B	562	LEU
1	B	575	ASP
1	B	577	VAL
1	B	581	LEU
1	B	660	LEU
1	B	681	ILE
1	B	785	LEU
1	B	850	TRP
1	B	885	ARG
1	B	914	THR
1	B	924	LYS
1	B	934	GLN
1	C	95	LEU
1	C	175	ARG

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Mol	Chain	Res	Type
1	C	209	ARG
1	C	261	THR
1	C	277	ASN
1	C	303	LEU
1	C	305	LYS
1	C	322	TRP
1	C	366	MET
1	C	395	LYS
1	C	413	LEU
1	C	478	LEU
1	C	526	LEU
1	C	559	THR
1	C	575	ASP
1	C	577	VAL
1	C	694	GLU
1	C	743	CYS
1	C	752	ARG
1	C	783	ASP
1	C	790	GLN
1	C	850	TRP
1	C	924	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	96	HIS
1	A	98	HIS
1	A	125	HIS
1	A	128	GLN
1	A	160	HIS
1	A	181	GLN
1	A	277	ASN
1	A	306	GLN
1	A	391	HIS
1	A	527	GLN
1	A	634	ASN
1	A	641	ASN
1	A	645	GLN
1	A	698	GLN
1	A	745	GLN
1	A	830	GLN

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Mol	Chain	Res	Type
1	A	934	GLN
1	B	96	HIS
1	B	125	HIS
1	B	160	HIS
1	B	181	GLN
1	B	277	ASN
1	B	357	HIS
1	B	391	HIS
1	B	446	ASN
1	B	634	ASN
1	B	698	GLN
1	B	745	GLN
1	B	925	ASN
1	B	934	GLN
1	C	68	HIS
1	C	96	HIS
1	C	125	HIS
1	C	128	GLN
1	C	160	HIS
1	C	277	ASN
1	C	357	HIS
1	C	391	HIS
1	C	446	ASN
1	C	546	GLN
1	C	564	HIS
1	C	628	HIS
1	C	634	ASN
1	C	698	GLN
1	C	745	GLN
1	C	810	ASN
1	C	830	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BES	A	1001	2	19,22,22	0.46	0	19,29,29	0.77	1 (5%)
4	NAG	A	5001	1,4	14,14,15	0.85	0	15,19,21	2.07	5 (33%)
4	NAG	A	5002	5,4	14,14,15	0.61	0	15,19,21	1.49	2 (13%)
5	BMA	A	5003	4,6	11,11,12	0.42	0	13,15,17	0.60	0
6	MAN	A	5004	5	11,11,12	0.59	0	13,15,17	0.86	0
6	MAN	A	5005	5	11,11,12	0.91	0	13,15,17	1.55	2 (15%)
4	NAG	A	6000	1	14,14,15	0.91	1 (7%)	15,19,21	1.41	2 (13%)
4	NAG	A	6001	1	14,14,15	1.27	2 (14%)	15,19,21	1.57	4 (26%)
3	BES	B	1001	2	19,22,22	0.48	0	19,29,29	0.84	1 (5%)
4	NAG	B	5001	1,4	14,14,15	0.74	0	15,19,21	1.18	1 (6%)
4	NAG	B	5002	4	14,14,15	0.63	0	15,19,21	1.59	2 (13%)
4	NAG	B	6000	1	14,14,15	0.64	0	15,19,21	0.99	1 (6%)
3	BES	C	1001	2	19,22,22	0.43	0	19,29,29	0.88	1 (5%)
4	NAG	C	5001	1,4	14,14,15	1.06	3 (21%)	15,19,21	1.96	6 (40%)
4	NAG	C	5002	5,4	14,14,15	0.71	0	15,19,21	1.84	4 (26%)
5	BMA	C	5003	4,6	11,11,12	0.39	0	13,15,17	0.50	0
6	MAN	C	5004	5	11,11,12	0.45	0	13,15,17	0.80	0
6	MAN	C	5005	5	11,11,12	0.77	0	13,15,17	1.01	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BES	A	1001	2	-	0/20/24/24	0/1/1/1
4	NAG	A	5001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	5002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	5003	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	5004	5	-	0/2/19/22	0/1/1/1
6	MAN	A	5005	5	-	0/2/19/22	0/1/1/1
4	NAG	A	6000	1	-	0/6/23/26	0/1/1/1
4	NAG	A	6001	1	1/1/5/7	0/6/23/26	0/1/1/1
3	BES	B	1001	2	-	0/20/24/24	0/1/1/1
4	NAG	B	5001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	5002	4	-	0/6/23/26	0/1/1/1
4	NAG	B	6000	1	-	0/6/23/26	0/1/1/1
3	BES	C	1001	2	-	0/20/24/24	0/1/1/1
4	NAG	C	5001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	5002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	C	5003	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	5004	5	-	0/2/19/22	0/1/1/1
6	MAN	C	5005	5	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5001	NAG	C4-C3	-2.12	1.47	1.52
4	C	5001	NAG	O4-C4	-2.10	1.38	1.43
4	C	5001	NAG	O5-C1	2.02	1.47	1.43
4	A	6000	NAG	O5-C1	2.27	1.47	1.43
4	A	6001	NAG	O5-C1	2.67	1.48	1.43
4	A	6001	NAG	C1-C2	3.23	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5001	NAG	O4-C4-C3	-4.42	100.75	110.36
4	A	6001	NAG	O5-C1-C2	-3.60	106.46	111.47
4	A	5001	NAG	O3-C3-C4	-3.57	102.59	110.36
4	B	5002	NAG	C4-C3-C2	-3.54	105.84	111.02
4	C	5002	NAG	C4-C3-C2	-3.51	105.88	111.02
4	A	5001	NAG	O4-C4-C3	-3.40	102.96	110.36
6	A	5005	MAN	C6-C5-C4	-3.40	105.05	113.00
4	C	5002	NAG	C1-O5-C5	-3.31	107.60	112.17
4	A	5001	NAG	C3-C4-C5	-3.30	104.41	110.22
4	A	5001	NAG	O3-C3-C2	-3.04	102.88	109.39
4	A	5002	NAG	C4-C3-C2	-2.90	106.77	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6001	NAG	C6-C5-C4	-2.88	106.26	113.00
3	C	1001	BES	C4-N1-C3	-2.80	118.88	123.16
4	A	6000	NAG	O5-C1-C2	-2.66	107.77	111.47
4	C	5001	NAG	C3-C4-C5	-2.55	105.72	110.22
3	B	1001	BES	C4-N1-C3	-2.28	119.67	123.16
6	C	5005	MAN	C6-C5-C4	-2.28	107.66	113.00
4	C	5001	NAG	O3-C3-C4	-2.28	105.39	110.36
6	A	5005	MAN	O3-C3-C4	-2.24	105.49	110.36
4	C	5001	NAG	O3-C3-C2	-2.11	104.87	109.39
3	A	1001	BES	C7-C6-C1	-2.03	109.17	113.50
4	C	5002	NAG	O4-C4-C3	-2.01	105.99	110.36
4	A	6001	NAG	C4-C3-C2	-2.00	108.08	111.02
4	C	5001	NAG	O4-C4-C5	-2.00	104.24	109.28
4	B	6000	NAG	C1-O5-C5	2.05	114.99	112.17
4	A	5001	NAG	C1-C2-N2	2.15	114.16	110.49
4	C	5001	NAG	C1-C2-N2	2.40	114.59	110.49
4	A	6001	NAG	C1-O5-C5	2.71	115.90	112.17
4	B	5001	NAG	C1-O5-C5	2.78	115.99	112.17
4	A	6000	NAG	C1-O5-C5	3.40	116.85	112.17
4	A	5002	NAG	C6-C5-C4	4.05	122.48	113.00
4	B	5002	NAG	C6-C5-C4	4.14	122.70	113.00
4	C	5002	NAG	C6-C5-C4	4.24	122.93	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	6001	NAG	C1
4	C	5001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	BES	2	0
4	A	5001	NAG	3	0
6	A	5004	MAN	1	0
4	A	6001	NAG	1	0
3	B	1001	BES	10	0
4	B	5001	NAG	1	0
3	C	1001	BES	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5002	NAG	1	0
6	C	5005	MAN	1	0

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	818/921 (88%)	-0.23	21 (2%) 56 37	26, 57, 133, 238	11 (1%)
1	B	821/921 (89%)	-0.15	36 (4%) 35 21	24, 57, 130, 223	11 (1%)
1	C	818/921 (88%)	-0.25	27 (3%) 47 30	28, 57, 130, 223	12 (1%)
All	All	2457/2763 (88%)	-0.21	84 (3%) 46 29	24, 57, 131, 238	34 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	SER	9.7
1	B	558	ASP	8.8
1	B	794	SER	8.4
1	B	557	PRO	8.3
1	B	827	ILE	7.4
1	B	339	SER	7.4
1	B	825	ASP	7.4
1	B	826	LYS	7.2
1	A	829	THR	5.9
1	C	794	SER	5.7
1	B	829	THR	5.5
1	B	792	SER	4.7
1	C	791	PHE	4.6
1	C	907	CYS	4.6
1	C	793	LEU	4.5
1	B	911	THR	4.5
1	B	556	ALA	4.4
1	A	889	GLU	4.3
1	B	824	GLY	4.2
1	C	762	SER	4.2
1	A	857	TRP	4.2
1	C	792	SER	4.2
1	A	339	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	757	SER	4.1
1	B	338	LYS	3.8
1	C	558	ASP	3.8
1	B	791	PHE	3.8
1	B	790	GLN	3.8
1	B	908	VAL	3.7
1	C	908	VAL	3.7
1	C	824	GLY	3.5
1	C	789	TYR	3.5
1	B	862	GLN	3.5
1	B	828	LYS	3.4
1	A	907	CYS	3.4
1	A	832	PHE	3.3
1	C	829	THR	3.3
1	A	794	SER	3.3
1	B	912	ILE	3.2
1	C	869	SER	3.2
1	B	759	GLY	3.1
1	B	337	GLU	3.1
1	A	871	ILE	3.0
1	A	851	GLN	2.8
1	A	415	SER	2.8
1	B	855	LYS	2.7
1	C	110	GLY	2.7
1	C	825	ASP	2.6
1	A	862	GLN	2.5
1	B	858	ASN	2.5
1	B	336	ALA	2.4
1	B	891	VAL	2.4
1	B	784	PHE	2.4
1	A	827	ILE	2.4
1	A	888	LEU	2.4
1	A	892	LYS	2.4
1	B	613	GLU	2.4
1	B	863	LYS	2.3
1	B	485	ILE	2.3
1	C	860	LEU	2.3
1	C	760	ASN	2.3
1	B	798	LYS	2.3
1	C	858	ASN	2.3
1	C	485	ILE	2.3
1	C	892	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	830	GLN	2.3
1	B	140	LEU	2.2
1	A	558	ASP	2.2
1	C	857	TRP	2.2
1	C	909	GLN	2.2
1	B	755	LYS	2.2
1	B	871	ILE	2.2
1	B	415	SER	2.2
1	A	890	GLU	2.2
1	A	752	ARG	2.2
1	B	868	SER	2.1
1	C	415	SER	2.1
1	C	850	TRP	2.1
1	A	362	ASN	2.1
1	A	789	TYR	2.0
1	C	911	THR	2.0
1	A	483	ALA	2.0
1	A	342	SER	2.0
1	B	316	SER	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	BES	A	1001	22/22	0.79	0.45	5.06	86,184,208,217	0
3	BES	C	1001	22/22	0.82	0.37	3.86	79,178,213,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BES	B	1001	22/22	0.88	0.38	3.50	121,167,185,218	0
6	MAN	C	5004	11/12	0.84	0.24	1.54	75,95,103,110	0
4	NAG	C	5001	14/15	0.90	0.19	1.43	20,79,110,127	0
4	NAG	A	5001	14/15	0.89	0.21	1.11	49,90,110,161	0
4	NAG	B	5001	14/15	0.91	0.21	1.00	50,93,110,139	0
2	ZN	B	1000	1/1	0.99	0.11	-0.88	38,38,38,38	0
2	ZN	C	1000	1/1	0.99	0.12	-0.93	38,38,38,38	0
2	ZN	A	1000	1/1	0.99	0.13	-1.25	40,40,40,40	0
4	NAG	B	6000	14/15	0.74	0.28	-	59,128,146,153	0
4	NAG	A	6000	14/15	0.82	0.19	-	76,119,141,145	0
4	NAG	C	5002	14/15	0.86	0.34	-	47,135,257,284	0
5	BMA	A	5003	11/12	0.89	0.17	-	51,86,129,131	0
4	NAG	A	5002	14/15	0.88	0.18	-	60,85,108,108	0
4	NAG	B	5002	14/15	0.75	0.25	-	118,161,189,212	0
6	MAN	C	5005	11/12	0.81	0.35	-	86,142,212,223	0
4	NAG	A	6001	14/15	0.74	0.17	-	72,140,150,153	0
6	MAN	A	5004	11/12	0.56	0.34	-	111,168,187,189	0
5	BMA	C	5003	11/12	0.85	0.26	-	43,135,191,223	0
6	MAN	A	5005	11/12	0.83	0.30	-	33,95,172,209	0

6.5 Other polymers ⓘ

There are no such residues in this entry.