Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:33 AM GMT

PDB ID	:	3MDJ
Title	:	ER Aminopeptidase, ERAP1, Bound to the Zinc Aminopeptidase Inhibitor, Bestatin
Authors	:	Nguyen, T.T.; Stern, L.J.
Deposited on	:	2010-03-30
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

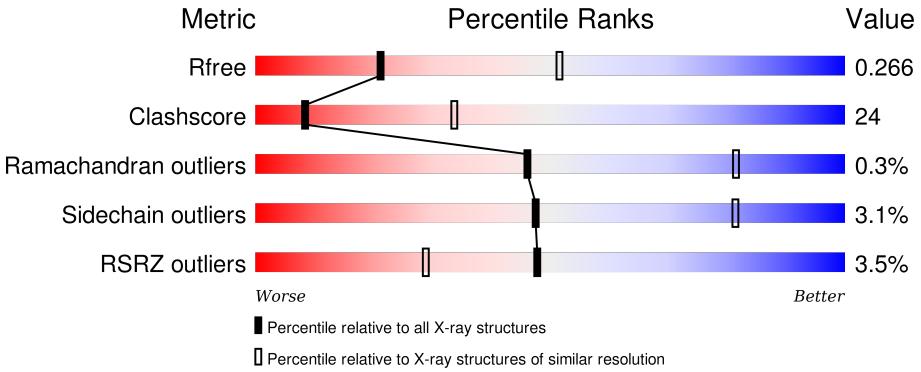
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (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 <=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	2% 51% 36% • 11%
1	B	921	4% 54% 33% • 11%
1	C	921	3% 50% 38% • 11%

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	C	5001	X	-	-	-
5	NAG	A	6001	X	-	-	-

2 Entry composition (i)

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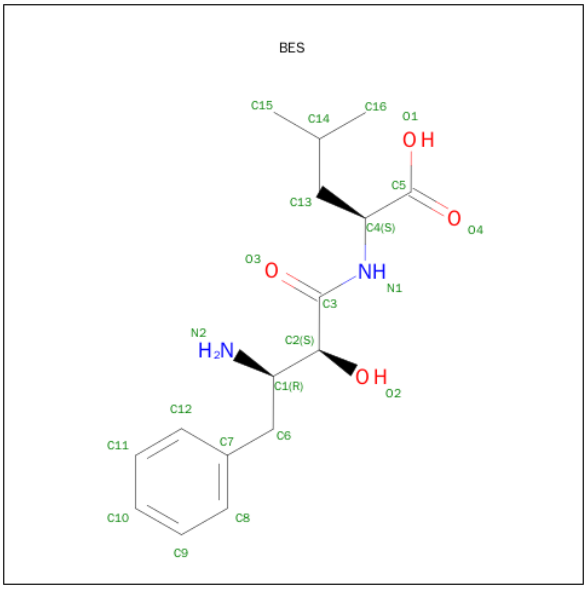
Chain	Residue	Modelled	Actual	Comment	Reference
C	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08

- 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: $C_{16}H_{24}N_2O_4$).

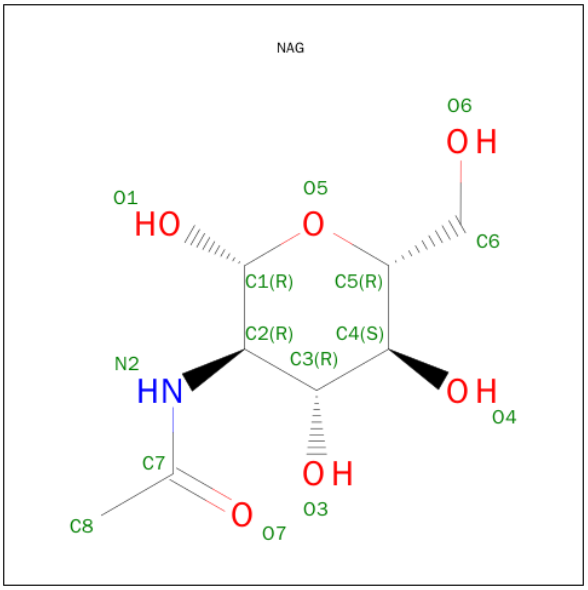


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 22 16 2 4	0	0
3	B	1	Total C N O 22 16 2 4	0	0
3	C	1	Total C N O 22 16 2 4	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total C N O 61 34 2 25	0	0
4	C	5	Total C N O 61 34 2 25	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

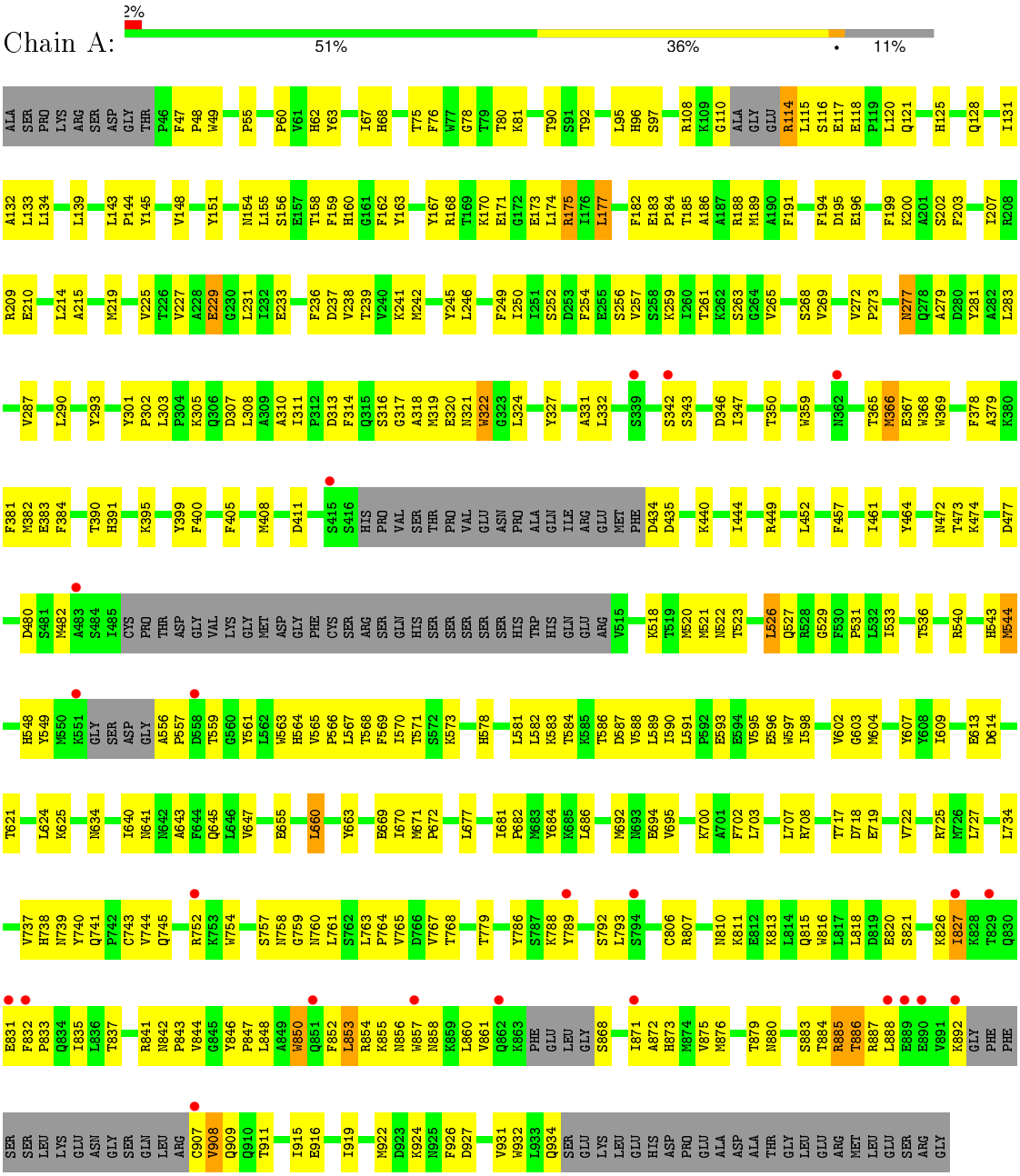
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total C N O 28 16 2 10	0	0

3 Residue-property plots (i)

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

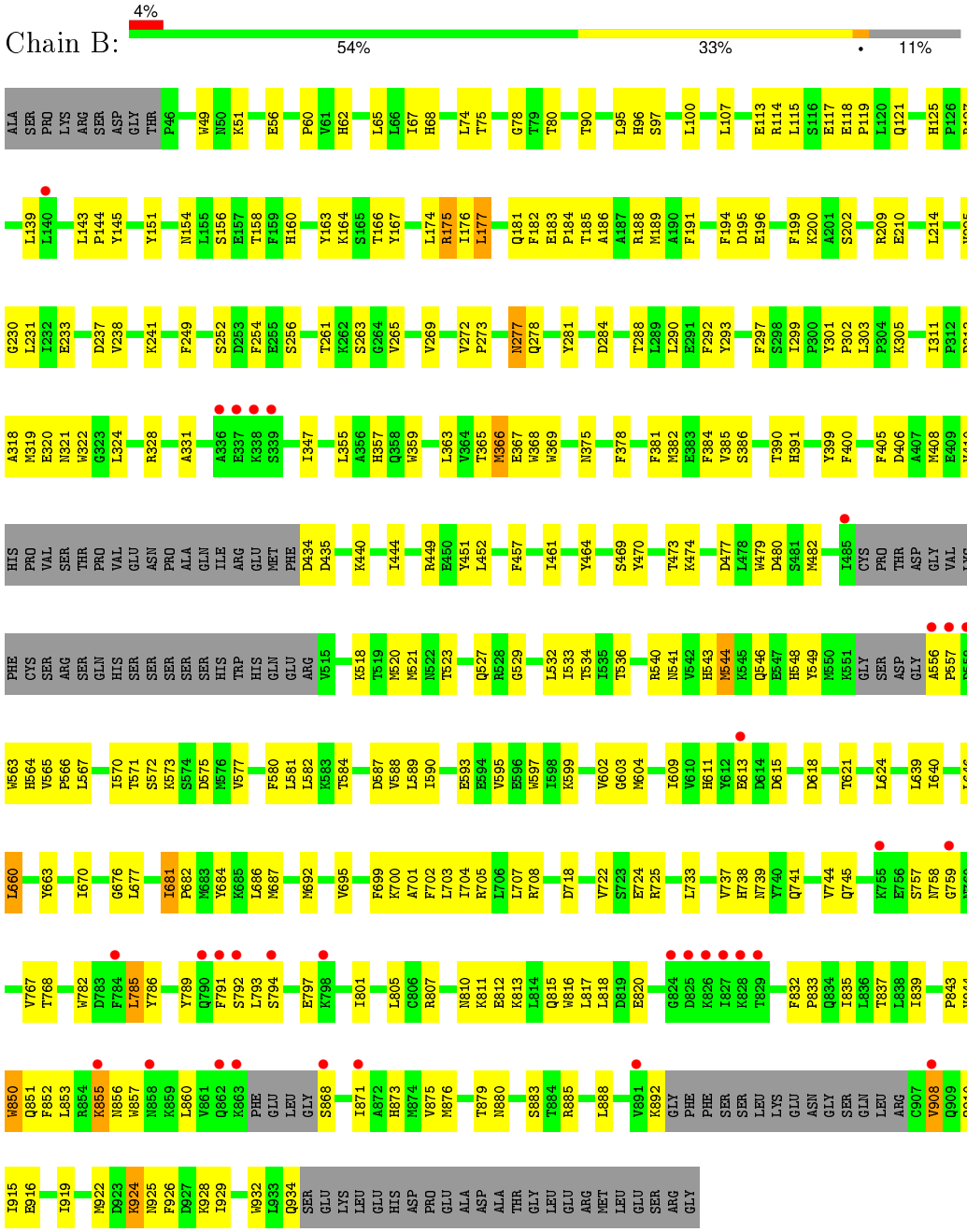
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain A:



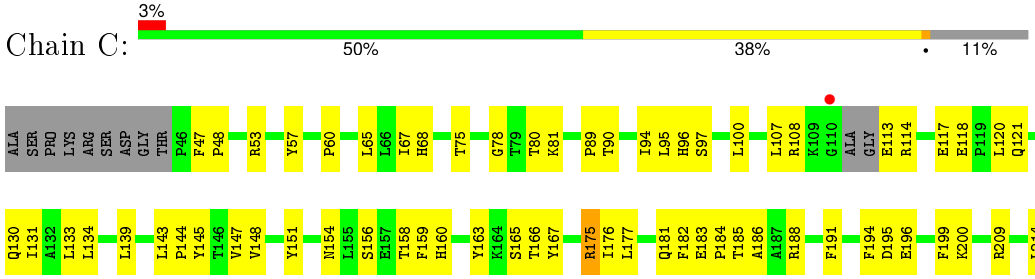
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

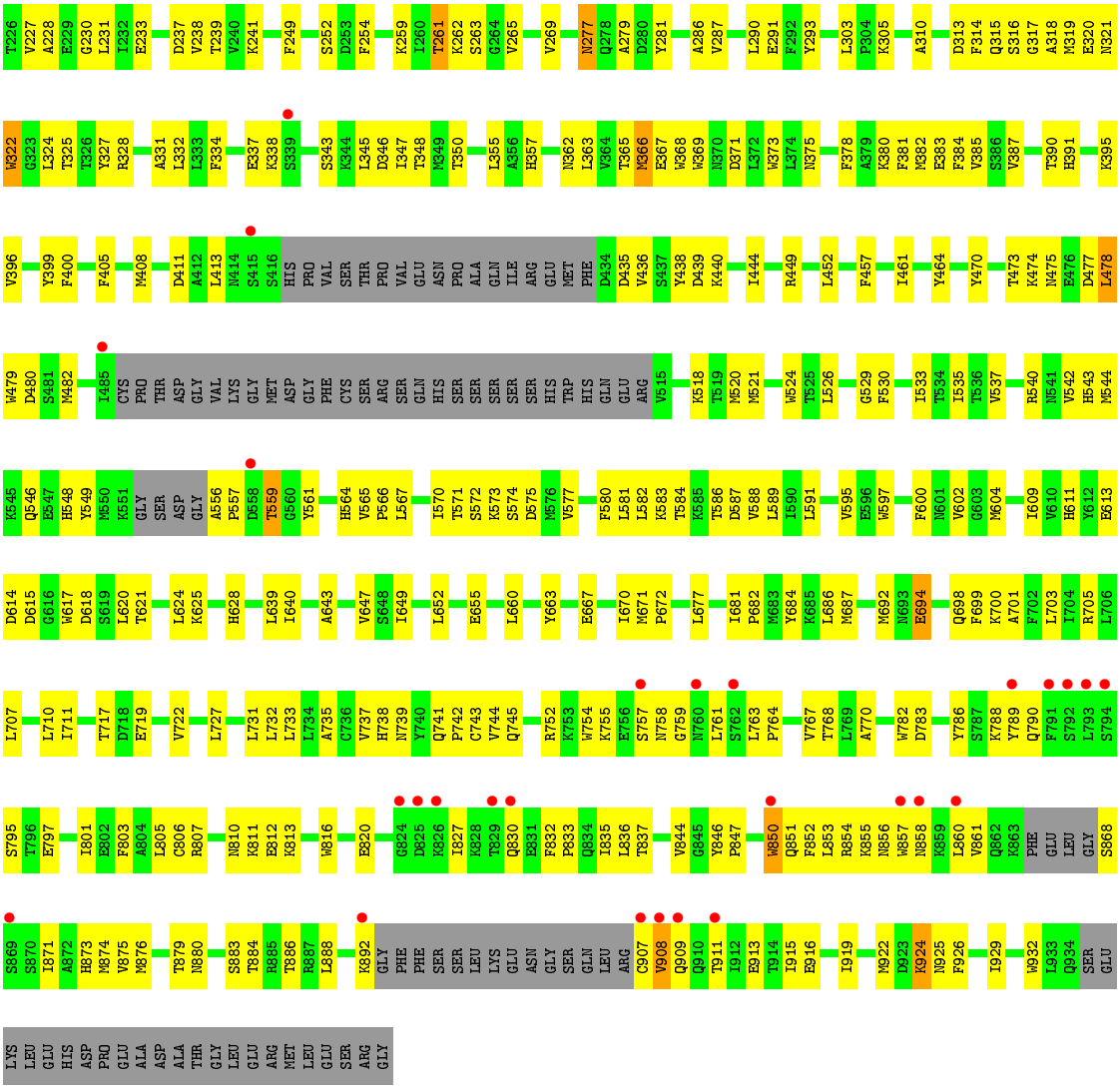
Chain B:



• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain C:




T226 V227 A228 E229 G230 L231 I232 E233 D237 V238 T239 V240 K241 F249 S252 D253 F254 K259 I260 T261 K262 S263 G264 V265 V269 N277 Q278 A279 D280 Y281 A286 V287 L290 E291 F292 Y293 L303 P304 K305 A310 D313 F314 Q315 S316 G317 A318 M319 E320 N321
W322 G323 L324 T325 T326 Y327 R328 A331 L332 L333 F334 E337 K338 S339 S343 K344 L345 D346 I347 T348 M349 T350 L355 A356 H357 N362 L363 V364 T365 M366 E367 W368 V369 N370 D371 L372 W373 L374 N375 F378 A379 K380 F381 M382 E383 F384 V385 S386 V387 T390 H391 K395
V396 Y399 F400 F405 M408 D411 A412 L413 N414 S415 S416 HIS PRO VAL SER THR PRO VAL GLU ASN PRO ALA GLN ILE ARG GLU MET PHE D434 D435 V436 S437 Y438 D439 K440 I444 R449 L452 F457 I461 Y464 Y470 T473 K474 N475 E476 D477 L478
W479 D480 S481 M482 I485 CYS PRO THR ASP GLY VAL LYS GLY MET ASP GLY PHE CYS SER ARG SER GLN HIS SER SER SER SER HIS TRP HIS GLN GLU ARG V515 K518 T519 M520 M521 W524 T525 L526 G529 P530 I533 T534 I535 T536 V537 R540 N541 V542 H543 M544
K545 Q546 E547 H548 Y549 M550 K551 GLY SER ASP GLY A556 P557 D558 T559 G560 V561 H564 V565 P566 L567 I570 T571 S572 K573 S574 D575 M576 V577 F580 L581 L582 K583 T584 K585 T586 D587 V588 L589 I590 L591 V595 E596 W597 F600 M601 V602 G603 M604 I609 V610 H611 Y612 E613
D614 D615 G616 W617 D618 S619 L620 T621 L624 K625 H628 L639 I640 A643 V647 S648 I649 L652 E655 L660 Y663 E667 I670 M671 P672 L677 I681 P682 M683 Y684 K685 L686 M687 M692 N693 E694 Q698 F699 K700 A701 F702 L703 I704 R705 L706
L707 L710 I711 T717 D718 E719 V722 L727 L731 L732 L733 L734 A735 C736 V737 H738 N739 Y740 Q741 P742 C743 V744 Q745 R752 K753 W754 K755 E756 S757 N758 G759 N760 L761 S762 L763 P764 V767 T768 L769 A770 W782 D783 Y786 S787 K788 Y789 Q790 F791 S792 L793 S794
S795 T796 E797 I801 E802 F803 A804 L805 C806 R807 N810 K811 E812 K813 W816 E820 G824 D825 K826 I827 K828 T829 Q830 E831 F832 P833 Q834 I835 L836 T837 V844 G845 Y846 P847 W850 Q851 F852 L853 R854 K855 N856 W857 N858 K859 L860 V861 Q862 K863 PHE GLU LEU GLY S868
S869 S870 I871 A872 H873 M874 V875 M876 T879 N880 S883 T884 R885 T886 R887 L888 K892 GLY PHE PHE SER SER LEU LYS GLU ASN GLY SER GLN LEU ARG C907 Y908 Q909 Q910 T911 I912 E913 T914 I915 E916 I919 M922 D923 K924 N925 F926 I929 W932 L933 Q934 SER GLU
LYS LEU GLU HIS ASP PRO GLU ALA ASP ALA THR GLY LEU GLU ARG MET LEU GLU SER ARG GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.03Å 234.63Å 95.86Å 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
$< I/\sigma(I) >$ [1]	1.53 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.199 , 0.264 0.200 , 0.266	Depositor DCC
R_{free} test set	3208 reflections (5.30%)	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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 63770 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

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
4	C	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	5001	NAG	C1

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	61	0	52	4	0
4	C	61	0	52	1	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
6	B	28	0	25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:227:VAL:HG21	1:C:233:GLU:HB2	1.50	0.93
1:B:544:MET:HG3	1:B:582:LEU:HD23	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
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:C:810:ASN:HD22	1:C:813:LYS:HD3	1.44	0.83
1:B:185:THR:HG23	1:B:188:ARG:CZ	2.07	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:B:182:PHE:HA	1:B:186:ALA:HB3	1.58	0.82
1:A:314:PHE:CE2	1:A:316:SER:HB2	2.14	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:C:621:THR:HG22	1:C:660:LEU:CD1	2.10	0.80
1:A:872:ALA:O	1:A:875:VAL:HG12	1.81	0.80
1:A:763:LEU:HG	1:A:768:THR:HG22	1.63	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:875:VAL:CG1	1:B:908:VAL:HG11	2.12	0.79
1:B:473:THR:HG23	1:B:477:ASP:HB2	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:883:SER:HB2	1:B:922:MET:HG3	1.67	0.77
1:A:350:THR:HA	3:A:1001:BES:H162	1.66	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
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:319:MET:SD	1:B:320:GLU:OE1	2.44	0.76
1:B:227:VAL:HG21	1:B:233:GLU:HB2	1.66	0.76
1:C:856:ASN:O	1:C:860:LEU:HB2	1.86	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: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:C:319:MET:CE	3:C:1001:BES:HN21	1.98	0.75
1:B:185:THR:O	1:B:185:THR:HG22	1.86	0.75
1:A:816:TRP:O	1:A:820:GLU:HG2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:THR:HG22	1:C:176:ILE:HD13	1.72	0.72
1:B:60:PRO:HG3	1:B:194:PHE:CD2	2.25	0.72
1:C:640:ILE:CD1	1:C:663:TYR:HE2	1.98	0.71
1:A:581:LEU:CD1	1:A:583:LYS:HG3	2.20	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
1:A:367:GLU:OE1	1:A:474:LYS:HE3	1.90	0.70
1:B:737:VAL:HG13	1:B:807:ARG:NH2	2.06	0.70
1:B:580:PHE:HZ	1:B:587:ASP:OD2	1.74	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:888:LEU:HD21	1:A:915:ILE:CG2	2.22	0.69
1:A:571:THR:CG2	1:A:573:LYS:H	2.01	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:C:228:ALA:HB3	1:C:231:LEU:HB2	1.75	0.68
1:B:549:TYR:CD1	1:B:609:ILE:HD11	2.27	0.68
1:A:681:ILE:HB	1:A:682:PRO:HD3	1.74	0.68
1:B:399:TYR:OH	1:B:722:VAL:HB	1.92	0.68
1:B:390:THR:HG22	1:B:391:HIS:CD2	2.28	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:C:852:PHE:CZ	1:C:856:ASN:ND2	2.61	0.67
1:B:381:PHE:HZ	1:B:449:ARG:HD2	1.58	0.67
1:A:200:LYS:HB2	1:A:241:LYS:HE2	1.75	0.67
1:C:571:THR:HG22	1:C:573:LYS:N	2.10	0.67
1:B:49:TRP:CH2	1:B:51:LYS:HD2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	5: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: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:B:464:TYR:OH	1:B:473:THR:HG21	1.96	0.65
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:A:200:LYS:CE	1:A:365:THR:HG22	2.26	0.65
1:C:671:MET:HB3	1:C:672:PRO:HD3	1.77	0.65
1:B:559:THR:HG22	1:B:561:TYR:H	1.62	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:763:LEU:CG	1:A:768:THR:HG22	2.27	0.65
1:A:540:ARG:HD2	1:A:591:LEU:O	1.96	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:A:832:PHE:N	1:A:833:PRO:HD2	2.12	0.65
1:B:80:THR:HG21	1:B:191:PHE:HB2	1.79	0.64
1:A:80:THR:HG21	1:A:191:PHE:HB2	1.80	0.64
1:C:121:GLN:HB3	1:C:134:LEU:HB2	1.78	0.64
1:A:916:GLU:HA	1:A:919:ILE:HD12	1.80	0.64
1:A:390:THR:HG22	1:A:391:HIS:CD2	2.33	0.64
1:C:156:SER:OG	1:C:158:THR:HG22	1.97	0.64
1:A:883:SER:HB2	1:A:922:MET:HG3	1.80	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:B:316:SER:N	1:B:317:GLY:HA2	2.11	0.64
1:A:533:ILE:CD1	1:A:567:LEU:HD21	2.27	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:B:700:LYS:HD3	1:B:738:HIS:HD2	1.62	0.64
1:A:259:LYS:HD3	1:A:287:VAL:HG21	1.80	0.64
1:B:181:GLN:HE22	1:B:319:MET:CE	2.11	0.64
1:A:316:SER:N	1:A:317:GLY:HA2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:PRO:O	1:C:768:THR:HG23	1.98	0.63
1:C:581:LEU:HD12	1:C:583:LYS:HG3	1.80	0.63
1:B:167:TYR:CE1	1:B:175:ARG:HB2	2.34	0.63
1:A:108:ARG:HG2	1:A:117:GLU:HG3	1.79	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
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:700:LYS:HD3	1:C:738:HIS:CD2	2.34	0.63
1:C:97:SER:CB	1:C:131:ILE:HD11	2.28	0.63
1:C:875:VAL:HG12	1:C:908:VAL:HG11	1.81	0.63
1:A:200:LYS:HB3	1:A:241:LYS:HG2	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:C:700:LYS:HD3	1:C:738:HIS:HD2	1.64	0.62
1:B:640:ILE:HD11	1:B:676:GLY:HA2	1.81	0.62
1:A:677:LEU:HD21	1:A:707:LEU:HD11	1.81	0.62
1:C:57:TYR:CE1	1:C:90:THR:HG21	2.34	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:C:692:MET:SD	1:C:926:PHE:CZ	2.93	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: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:B:565:VAL:CG1	1:B:582:LEU:HB3	2.30	0.61
1:A:670:ILE:HD13	1:A:727:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:318:ALA:O	3:C:1001:BES:H2	2.00	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:B:261:THR:HG23	1:B:263:SER:N	2.16	0.60
1:A:464:TYR:OH	1:A:473:THR:HG21	2.00	0.60
1:A:185:THR:HG23	1:A:188:ARG:NH2	2.16	0.60
1:A:581:LEU:HD12	1:A:583:LYS:HG3	1.81	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:A:115:LEU:HD12	1:A:116:SER:H	1.67	0.60
1:C:754:TRP:NE1	1:C:759:GLY:HA2	2.16	0.60
1:B:480:ASP:OD1	1:B:518:LYS:HE2	2.01	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:B:114:ARG:HA	1:B:117:GLU:CG	2.32	0.60
1:A:595:VAL:HG12	1:A:597:TRP:H	1.66	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:67:ILE:HD13	1:B:249:PHE:CZ	2.36	0.60
1:B:527:GLN:OE1	1:B:563:TRP:NE1	2.34	0.60
1:B:571:THR:HG23	1:B:595:VAL:HG11	1.84	0.60
1:B:367:GLU:OE1	1:B:474:LYS:HE3	2.01	0.60
1:C:183:GLU:HB3	1:C:319:MET:HE3	1.82	0.59
1:B:757:SER:HB3	1:B:759:GLY:N	2.16	0.59
1:B:544:MET:HG3	1:B:582:LEU:CD2	2.27	0.59
1:A:703:LEU:HD21	1:A:734:LEU:HD21	1.84	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:588:VAL:HG12	1:A:589:LEU:H	1.67	0.59
1:A:531:PRO:HB3	1:A:563:TRP:CE3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:LEU:O	1:B:663:TYR:HD2	1.86	0.59
1:B:384:PHE:CE1	1:B:400:PHE:HB2	2.37	0.59
1:C:832:PHE:N	1:C:833:PRO:HD2	2.18	0.59
1:B:807:ARG:HH12	1:B:843:PRO:HD2	1.68	0.59
1:A:660:LEU:O	1:A:663:TYR:HD2	1.85	0.59
1:A:293:TYR:HE2	1:A:382:MET:HG3	1.67	0.59
1:B:565:VAL:HG12	1:B:582:LEU:HB3	1.85	0.59
1:B:166:THR:HG22	1:B:176:ILE:HD13	1.84	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: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:B:115:LEU:HD22	1:B:115:LEU:N	2.18	0.58
1:A:571:THR:HG23	1:A:595:VAL:CG1	2.34	0.58
1:B:807:ARG:NH1	1:B:843:PRO:HD2	2.19	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:78:GLY:HA3	1:B:151:TYR:CZ	2.38	0.58
1:A:523:THR:O	1:A:527:GLN:HB2	2.03	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:C:588:VAL:HG12	1:C:589:LEU:N	2.19	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: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:588:VAL:CG1	1:A:589:LEU:N	2.66	0.57
1:A:559:THR:CG2	1:A:561:TYR:H	2.16	0.57
1:B:846:TYR:N	1:B:847:PRO:CD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:660:LEU:O	1:C:663:TYR:HD2	1.87	0.57
1:B:852:PHE:CZ	1:B:856:ASN:ND2	2.72	0.57
1:C:464:TYR:OH	1:C:473:THR:HG21	2.05	0.57
1:A:717:THR:OG1	1:A:719:GLU:HG2	2.05	0.57
1:A:68:HIS:HE1	1:A:231:LEU:HD21	1.70	0.57
1:B:681:ILE:HB	1:B:682:PRO:HD3	1.86	0.57
1:B:615:ASP:HB2	1:B:618:ASP:HB2	1.85	0.57
1:A:786:TYR:O	1:A:789:TYR:HB3	2.05	0.57
1:A:261:THR:HG23	1:A:263:SER:H	1.70	0.56
1:A:588:VAL:CG1	1:A:589:LEU:H	2.17	0.56
1:A:237:ASP:OD1	1:A:238:VAL:N	2.37	0.56
1:C:733:LEU:O	1:C:737:VAL:HG23	2.05	0.56
1:B:523:THR:O	1:B:563:TRP:CD1	2.58	0.56
1:A:739:ASN:HA	1:A:744:VAL:HG21	1.87	0.56
1:C:261:THR:HG22	1:C:265:VAL:N	2.19	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:B:139:LEU:HD22	1:B:145:TYR:HE1	1.70	0.56
1:C:408:MET:HG2	1:C:530:PHE:CE2	2.40	0.56
1:B:319:MET:CE	3:B:1001:BES:HN21	2.19	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:810:ASN:CB	1:B:813:LYS:HD2	2.35	0.56
1:B:621:THR:CG2	1:B:660:LEU:HG	2.25	0.56
1:A:754:TRP:NE1	1:A:759:GLY:HA2	2.20	0.56
1:C:156:SER:HB3	1:C:163:TYR:HB3	1.88	0.56
1:C:699:PHE:O	1:C:703:LEU:HD13	2.05	0.56
1:C:559:THR:HG22	1:C:561:TYR:H	1.71	0.56
1:A:741:GLN:HE21	1:A:745:GLN:HE21	1.52	0.56
1:C:80:THR:HG21	1:C:191:PHE:HB2	1.86	0.56
1:C:757:SER:N	1:C:758:ASN:HA	2.21	0.56
1:B:293:TYR:HE2	1:B:382:MET:HG3	1.70	0.56
1:C:757:SER:HB3	1:C:759:GLY:N	2.20	0.56
1:B:876:MET:O	1:B:880:ASN:HB2	2.05	0.56
1:B:281:TYR:CD2	1:B:347:ILE:HD11	2.40	0.56
1:A:272:VAL:HG13	1:A:273:PRO:HD2	1.86	0.56
1:C:281:TYR:CD2	1:C:347:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:621:THR:O	1:A:625:LYS:HG3	2.06	0.55
1:C:542:VAL:HB	1:C:589:LEU:HB3	1.88	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:B:49:TRP:CZ2	1:B:51:LYS:HD2	2.40	0.55
1:B:785:LEU:HD22	1:B:801:ILE:HG23	1.88	0.55
1:C:230:GLY:C	1:C:231:LEU:HD12	2.26	0.55
1:C:544:MET:HG3	1:C:582:LEU:CD2	2.36	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: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: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:853:LEU:O	1:A:857:TRP:HB2	2.06	0.55
1:A:621:THR:CG2	1:A:660:LEU:HG	2.35	0.55
1:C:811:LYS:HE2	1:C:844:VAL:HG13	1.88	0.55
1:B:62:HIS:HE1	1:B:238:VAL:HG13	1.71	0.55
1:A:837:THR:HG21	1:A:873:HIS:NE2	2.21	0.55
1:C:549:TYR:HE1	1:C:649:ILE:HD13	1.70	0.55
1:B:807:ARG:HH12	1:B:843:PRO:CD	2.19	0.55
1:B:457:PHE:CD1	1:B:482:MET:HE3	2.42	0.55
1:C:533:ILE:CD1	1:C:567:LEU:HD21	2.36	0.55
1:C:97:SER:HB3	1:C:131:ILE:HD11	1.87	0.55
1:C:699:PHE:CE2	1:C:703:LEU:HD11	2.42	0.55
1:B:797:GLU:O	1:B:801:ILE:HG13	2.07	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:B:185:THR:O	1:B:185:THR:CG2	2.54	0.54
1:A:327:TYR:CE1	1:A:350:THR:HG22	2.40	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:C:546:GLN:HE21	1:C:582:LEU:CD1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:MET:SD	1:B:566:PRO:HG3	2.48	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:C:707:LEU:O	1:C:711:ILE:HG13	2.07	0.54
1:B:811:LYS:HE2	1:B:844:VAL:CG1	2.38	0.54
1:B:793:LEU:HG	1:B:794:SER:OG	2.07	0.54
1:C:310:ALA:HB2	1:C:332:LEU:HD23	1.90	0.54
1:A:876:MET:O	1:A:880:ASN:HB2	2.07	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:C:803:PHE:CE2	1:C:807:ARG:HG3	2.43	0.53
1:B:640:ILE:HD11	1:B:676:GLY:CA	2.38	0.53
1:A:590:ILE:HG13	1:B:470:TYR:CG	2.42	0.53
1:B:588:VAL:CG1	1:B:589:LEU:N	2.71	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: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: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: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:A:76:PHE:HD1	1:A:155:LEU:HD12	1.73	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:C:444:ILE:HG22	1:C:521:MET:HE1	1.89	0.53
1:B:853:LEU:O	1:B:857:TRP:HB2	2.08	0.53
1:B:156:SER:HB3	1:B:163:TYR:HB3	1.90	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:C:611:HIS:CE1	1:C:617:TRP:HE1	2.27	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:C:185:THR:O	1:C:185:THR:CG2	2.56	0.53
1:B:580:PHE:CZ	1:B:587:ASP:OD2	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:CD2	1:A:347:ILE:HD11	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:C:343:SER:O	1:C:347:ILE:HG23	2.09	0.52
1:B:910:GLN:O	1:B:914:THR:HG22	2.09	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: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:A:63:TYR:CD1	1:A:203:PHE:CE1	2.97	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:261:THR:HG23	1:C:263:SER:N	2.21	0.52
1:B:230:GLY:C	1:B:231:LEU:HD12	2.30	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:C:60:PRO:HG3	1:C:194:PHE:CG	2.44	0.52
1:C:327:TYR:CD2	1:C:332:LEU:HD22	2.45	0.52
1:B:75:THR:HG22	1:B:154:ASN:OD1	2.10	0.52
1:A:120:LEU:HD13	1:A:133:LEU:HB3	1.92	0.52
1:C:117:GLU:O	1:C:118:GLU:HG3	2.08	0.51
1:C:684:TYR:HB3	1:C:699:PHE:CD2	2.45	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: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:B:183:GLU:HB3	1:B:319:MET:CE	2.40	0.51
1:A:582:LEU:CD1	1:A:584:THR:O	2.58	0.51
1:B:615:ASP:HB2	1:B:618:ASP:CG	2.31	0.51
1:B:68:HIS:HE1	1:B:231:LEU:HD21	1.75	0.51
1:A:405:PHE:CZ	1:A:604:MET:SD	3.03	0.51
1:B:532:LEU:HD11	1:B:646:LEU:HD21	1.92	0.51
1:A:655:GLU:HB2	1:A:932:TRP:CD1	2.45	0.51
1:C:237:ASP:OD1	1:C:238:VAL:N	2.43	0.51
1:A:110:GLY:HA3	1:A:114:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:THR:O	1:C:625:LYS:HG3	2.10	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:A:97:SER:HB2	1:A:131:ILE:HD11	1.91	0.51
1:C:670:ILE:HD13	1:C:727:LEU:HD22	1.92	0.51
1:A:308:LEU:N	1:A:308:LEU:HD12	2.26	0.51
1:A:565:VAL:HG12	1:A:582:LEU:HB3	1.93	0.51
1:C:595:VAL:HG12	1:C:597:TRP:H	1.76	0.51
1:C:322:TRP:CD2	1:C:362:ASN:HB3	2.46	0.51
1:A:170:LYS:HG3	1:A:171:GLU:OE2	2.10	0.51
1:C:367:GLU:OE1	1:C:474:LYS:HE3	2.10	0.51
1:A:533:ILE:HD11	1:A:565:VAL:HG11	1.93	0.50
1:A:408:MET:HE1	1:A:609:ILE:HG23	1.92	0.50
1:C:694:GLU:O	1:C:698:GLN:HG3	2.11	0.50
1:A:761:LEU:HD12	1:A:761:LEU:O	2.10	0.50
1:A:473:THR:CG2	1:A:474:LYS:N	2.74	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:A:844:VAL:HG12	1:A:844:VAL:O	2.10	0.50
1:B:357:HIS:CE1	1:B:375:ASN:ND2	2.80	0.50
1:C:586:THR:O	1:C:587:ASP:OD1	2.29	0.50
1:B:655:GLU:OE2	1:B:928:LYS:HD3	2.11	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:876:MET:O	1:C:880:ASN:HB2	2.11	0.50
1:C:812:GLU:O	1:C:816:TRP:HB2	2.11	0.50
1:A:277:ASN:HD22	1:A:277:ASN:N	2.10	0.50
1:A:573:LYS:HG3	1:A:595:VAL:HG22	1.92	0.50
1:A:842:ASN:OD1	1:A:843:PRO:HD2	2.11	0.50
1:C:682:PRO:O	1:C:686:LEU:HD13	2.11	0.50
1:A:757:SER:H	1:A:758:ASN:HA	1.76	0.50
1:C:368:TRP:CG	1:C:369:TRP:N	2.79	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:549:TYR:CE1	1:C:609:ILE:HD11	2.46	0.50
1:C:100:LEU:HD22	1:C:151:TYR:HD2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ASP:HB3	1:A:725:ARG:NH1	2.26	0.50
1:B:311:ILE:HB	1:B:314:PHE:HB2	1.92	0.50
1:C:737:VAL:CG1	1:C:807:ARG:NH2	2.75	0.50
1:B:523:THR:O	1:B:563:TRP:NE1	2.45	0.50
1:A:290:LEU:HD12	1:A:359:TRP:HH2	1.77	0.50
1:C:907:CYS:C	1:C:909:GLN:H	2.15	0.50
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:A:256:SER:HA	1:A:269:VAL:O	2.12	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:C:314:PHE:CE2	1:C:316:SER:CB	2.84	0.49
1:A:80:THR:HG23	1:A:151:TYR:CE1	2.36	0.49
1:A:440:LYS:HE3	1:A:607:TYR:CE2	2.48	0.49
1:B:479:TRP:CH2	1:B:521:MET:HE2	2.48	0.49
1:C:346:ASP:O	1:C:350:THR:HG23	2.12	0.49
1:B:875:VAL:HB	1:B:908:VAL:HG21	1.94	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:C:764:PRO:HB2	1:C:767:VAL:HG22	1.93	0.49
1:A:586:THR:O	1:A:587:ASP:OD1	2.31	0.49
1:C:262:LYS:HG3	1:C:291:GLU:OE2	2.12	0.49
1:B:125:HIS:CD2	1:B:127:ARG:HB3	2.47	0.49
1:C:643:ALA:O	1:C:647:VAL:HG23	2.12	0.49
1:C:183:GLU:HB3	1:C:319:MET:CE	2.42	0.49
1:B:366:MET:HG3	1:B:368:TRP:O	2.12	0.49
1:A:624:LEU:HD12	1:A:660:LEU:HD21	1.93	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:875:VAL:HG21	1:A:908:VAL:HG11	1.95	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:B:290:LEU:HD12	1:B:359:TRP:HH2	1.77	0.49
1:B:761:LEU:O	1:B:761:LEU:HD12	2.13	0.49
1:C:737:VAL:CG1	1:C:807:ARG:HH21	2.25	0.49
1:B:107:LEU:HD11	1:B:145:TYR:HB3	1.94	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:A:177:LEU:HD13	1:A:254:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLU:HG3	6:B:5001:NAG:H82	1.95	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:480:ASP:OD1	1:A:518:LYS:HE2	2.12	0.49
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
1:C:908:VAL:CG1	1:C:908:VAL:O	2.60	0.48
1:B:534:THR:HG22	1:B:613:GLU:HG2	1.95	0.48
1:A:200:LYS:HE2	1:A:365:THR:CG2	2.43	0.48
1:C:588:VAL:CG1	1:C:589:LEU:N	2.76	0.48
1:B:384:PHE:CE2	1:B:400:PHE:HD1	2.32	0.48
1:B:888:LEU:O	1:B:892:LYS:HG3	2.13	0.48
1:B:225:VAL:O	1:B:227:VAL:HG23	2.13	0.48
1:A:604:MET:HE1	1:A:634:ASN:HB3	1.95	0.48
1:C:78:GLY:HA3	1:C:151:TYR:CZ	2.48	0.48
1:A:47:PHE:HA	1:A:48:PRO:HD3	1.61	0.48
1:B:319:MET:HE2	3:B:1001:BES:C8	2.43	0.48
1:B:533:ILE:HD13	1:B:567:LEU:HD21	1.95	0.48
1:B:214:LEU:HD23	1:B:252:SER:O	2.14	0.48
1:C:350:THR:HA	3:C:1001:BES:H162	1.95	0.48
1:A:831:GLU:HG2	1:A:835:ILE:HD11	1.95	0.48
1:A:811:LYS:HE2	1:A:844:VAL:CG1	2.43	0.48
1:A:536:THR:HB	1:A:543:HIS:HB2	1.95	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:924:LYS:NZ	1:B:924:LYS:HB2	2.29	0.48
1:B:908:VAL:HG13	1:B:911:THR:OG1	2.14	0.48
1:B:571:THR:HG23	1:B:595:VAL:CG1	2.43	0.48
1:C:139:LEU:HD22	1:C:145:TYR:HE1	1.78	0.48
1:B:815:GLN:HA	1:B:818:LEU:HD12	1.96	0.48
1:B:319:MET:HE1	3:B:1001:BES:HN21	1.78	0.48
1:C:544:MET:CG	1:C:582:LEU:HD23	2.43	0.48
1:A:669:GLU:O	1:A:672:PRO:HD2	2.14	0.48
1:C:846:TYR:N	1:C:847:PRO:CD	2.76	0.48
1:C:325:THR:HG23	1:C:327:TYR:CE2	2.48	0.48
1:B:378:PHE:CE1	1:B:461:ILE:HD13	2.48	0.48
1:B:292:PHE:CZ	1:B:386:SER:HA	2.49	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:754:TRP:CE2	1:C:759:GLY:HA2	2.49	0.48
1:C:444:ILE:CG2	1:C:521:MET:HE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:682:PRO:O	1:B:686:LEU:HD13	2.14	0.47
1:B:615:ASP:HB2	1:B:618:ASP:CB	2.44	0.47
1:B:457:PHE:CD1	1:B:482:MET:CE	2.97	0.47
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:588:VAL:CG1	1:C:241:LYS:HD2	2.39	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:C:916:GLU:HA	1:C:919:ILE:HD12	1.96	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: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:202:SER:OG	1:A:238:VAL:CG1	2.61	0.47
1:A:569:PHE:CZ	1:A:589:LEU:HD21	2.50	0.47
1:B:588:VAL:CG1	1:B:589:LEU:H	2.28	0.47
1:A:115:LEU:HD12	1:A:116:SER:N	2.29	0.47
1:A:846:TYR:N	1:A:847:PRO:CD	2.77	0.47
1:A:826:LYS:O	1:A:827:ILE:HB	2.15	0.47
1:C:371:ASP:OD1	1:C:475:ASN:ND2	2.48	0.47
1:C:853:LEU:O	1:C:857:TRP:HB2	2.15	0.47
1:A:257:VAL:HG23	1:A:283:LEU:HD22	1.96	0.47
1:A:229:GLU:HA	1:A:229:GLU:OE1	2.15	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:B:532:LEU:HD12	1:B:609:ILE:O	2.15	0.47
1:A:246:LEU:CD2	1:A:320:GLU:HG2	2.45	0.47
1:C:53:ARG:HD3	1:C:368:TRP:CH2	2.50	0.47
1:B:200:LYS:CE	1:B:365:THR:HG22	2.45	0.47
1:C:624:LEU:O	1:C:628:HIS:HB3	2.15	0.47
1:A:159:PHE:CE1	1:A:313:ASP:HB3	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:334:PHE:HE1	1:C:338:LYS:HB3	1.79	0.46
1:A:692:MET:SD	1:A:926:PHE:CZ	3.08	0.46
1:C:227:VAL:HG21	1:C:233:GLU:CB	2.33	0.46
1:A:582:LEU:HD11	1:A:584:THR:O	2.14	0.46
1:C:888:LEU:HD11	1:C:919:ILE:CD1	2.44	0.46
1:C:733:LEU:HA	1:C:770:ALA:HB2	1.98	0.46
1:A:63:TYR:HB2	1:A:203:PHE:CD1	2.50	0.46
1:C:181:GLN:OE1	1:C:319:MET:HE3	2.15	0.46
1:B:314:PHE:HE2	1:B:317:GLY:C	2.19	0.46
1:C:757:SER:H	1:C:758:ASN:HA	1.81	0.46
1:C:133:LEU:HD13	1:C:147:VAL:HG11	1.97	0.46
1:A:384:PHE:CE2	1:A:400:PHE:HD1	2.34	0.46
1:A:565:VAL:HA	1:A:566:PRO:HD3	1.68	0.46
1:A:200:LYS:HE2	1:A:365:THR:HG22	1.98	0.46
1:B:297:PHE:O	1:B:299:ILE:HG13	2.15	0.46
1:B:763:LEU:CD2	1:B:768:THR:HG22	2.45	0.46
1:C:544:MET:HG3	1:C:582:LEU:HD21	1.98	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:C:281:TYR:HD2	1:C:347:ILE:HD11	1.80	0.46
1:C:806:CYS:SG	1:C:835:ILE:HG23	2.55	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:C:615:ASP:HB3	1:C:618:ASP:HB2	1.98	0.46
1:A:858:ASN:O	1:A:861:VAL:HG22	2.16	0.46
1:C:761:LEU:O	1:C:761:LEU:HD12	2.16	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: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:C:384:PHE:HE1	1:C:396:VAL:O	1.99	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:A:268:SER:HB2	1:A:307:ASP:OD1	2.16	0.46
1:C:196:GLU:HB2	1:C:199:PHE:HD2	1.80	0.46
1:A:641:ASN:O	1:A:645:GLN:HG3	2.15	0.46
1:A:875:VAL:HG22	1:A:908:VAL:HG11	1.97	0.45
1:A:269:VAL:HG11	1:A:279:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ILE:HG13	1:C:470:TYR:CG	2.52	0.45
1:B:868:SER:HA	1:B:871:ILE:HG12	1.97	0.45
1:C:879:THR:OG1	1:C:911:THR:HG21	2.16	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:827:ILE:HD11	1:C:830:GLN:HE21	1.81	0.45
1:C:319:MET:SD	1:C:320:GLU:CD	2.94	0.45
1:A:681:ILE:HG23	1:A:684:TYR:OH	2.17	0.45
1:A:261:THR:HG23	1:A:263:SER:N	2.31	0.45
1:A:888:LEU:O	1:A:892:LYS:HG3	2.16	0.45
1:B:876:MET:HG2	1:B:911:THR:OG1	2.17	0.45
1:B:227:VAL:HG21	1:B:233:GLU:CB	2.42	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:B:181:GLN:NE2	3:B:1001:BES:C9	2.80	0.45
1:A:640:ILE:HD11	1:A:663:TYR:CE2	2.52	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:694:GLU:HG2	1:A:695:VAL:N	2.30	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:C:667:GLU:HG2	1:C:672:PRO:HB2	1.99	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:A:434:ASP:OD1	1:A:435:ASP:N	2.48	0.45
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.79	0.45
1:C:655:GLU:HB3	1:C:932:TRP:CD1	2.52	0.45
1:C:582:LEU:HD11	1:C:584:THR:O	2.17	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:227:VAL:CG2	1:C:233:GLU:HB2	2.34	0.45
1:B:687:MET:SD	1:B:695:VAL:HG12	2.57	0.45
1:B:156:SER:HB3	1:B:163:TYR:CB	2.47	0.44
1:C:384:PHE:O	1:C:385:VAL:C	2.54	0.44
1:A:868:SER:HA	1:A:871:ILE:CD1	2.48	0.44
1:A:846:TYR:CD2	1:A:847:PRO:HD3	2.53	0.44
1:C:604:MET:HG2	1:C:604:MET:O	2.17	0.44
1:B:718:ASP:HB3	1:B:725:ARG:NH1	2.32	0.44
1:C:852:PHE:CE1	1:C:856:ASN:ND2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG22	1:A:132:ALA:N	2.32	0.44
1:C:647:VAL:HA	1:C:652:LEU:O	2.17	0.44
1:C:405:PHE:HZ	1:C:604:MET:SD	2.40	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
1:C:65:LEU:HD22	1:C:80:THR:CG2	2.48	0.44
1:A:215:ALA:HA	1:A:250:ILE:O	2.18	0.44
1:C:47:PHE:HA	1:C:48:PRO:HD3	1.62	0.44
1:B:185:THR:HG23	1:B:188:ARG:NE	2.33	0.44
1:C:876:MET:HG2	1:C:911:THR:OG1	2.18	0.44
1:A:185:THR:CG2	1:A:185:THR:O	2.63	0.44
1:B:411:ASP:OD1	1:B:529:GLY:N	2.51	0.44
1:A:49:TRP:CZ3	1:A:55:PRO:HG3	2.52	0.44
1:C:183:GLU:OE1	1:C:320:GLU:OE2	2.35	0.44
1:B:595:VAL:HG12	1:B:597:TRP:N	2.29	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:A:879:THR:OG1	1:A:911:THR:HG21	2.17	0.44
1:A:324:LEU:HG	1:A:324:LEU:O	2.18	0.44
1:B:74:LEU:HD13	1:B:164:LYS:HD3	2.00	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:A:613:GLU:HG3	1:A:614:ASP:H	1.83	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:227:VAL:CG2	1:A:233:GLU:HB2	2.38	0.43
1:C:537:VAL:HG22	1:C:542:VAL:HG22	1.99	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:A:139:LEU:HB3	1:A:145:TYR:CE1	2.53	0.43
1:C:797:GLU:O	1:C:801:ILE:HG13	2.18	0.43
1:C:277:ASN:HD22	1:C:277:ASN:N	2.16	0.43
1:B:160:HIS:CD2	1:B:186:ALA:HB2	2.54	0.43
1:C:367:GLU:OE1	1:C:474:LYS:CE	2.66	0.43
1:C:754:TRP:HA	1:C:757:SER:HB2	2.00	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:A:556:ALA:HB3	1:A:557:PRO:HD3	1.99	0.43
1:B:196:GLU:HB2	1:B:199:PHE:HD2	1.84	0.43
1:C:68:HIS:CE1	1:C:231:LEU:CD2	2.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ARG:HG2	1:A:708:ARG:NH1	2.34	0.43
1:C:457:PHE:CE2	1:C:461:ILE:CD1	3.01	0.43
1:C:125:HIS:CE1	1:C:128:GLN:NE2	2.87	0.43
1:A:314:PHE:HE2	1:A:316:SER:HB2	1.77	0.43
1:C:544:MET:SD	1:C:567:LEU:HD12	2.59	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:A:604:MET:HG2	1:A:604:MET:O	2.17	0.43
1:B:444:ILE:HG22	1:B:521:MET:HE1	2.01	0.43
1:A:907:CYS:C	1:A:909:GLN:H	2.22	0.43
1:B:739:ASN:HA	1:B:744:VAL:HG21	2.00	0.43
1:C:94:ILE:HD12	1:C:94:ILE:N	2.33	0.43
1:C:858:ASN:O	1:C:861:VAL:HG22	2.19	0.43
1:B:434:ASP:HB3	1:B:435:ASP:H	1.70	0.43
1:B:611:HIS:ND1	1:B:646:LEU:HD13	2.32	0.43
1:C:544:MET:SD	1:C:580:PHE:CD2	3.12	0.43
1:C:160:HIS:CD2	1:C:186:ALA:HB2	2.54	0.43
1:B:879:THR:OG1	1:B:911:THR:HG21	2.18	0.43
1:C:373:TRP:HA	1:C:438:TYR:CE2	2.53	0.43
1:B:405:PHE:CZ	1:B:604:MET:SD	3.12	0.43
1:A:368:TRP:CG	1:A:369:TRP:N	2.87	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:C:572:SER:OG	1:C:595:VAL:HG13	2.18	0.43
1:C:185:THR:CG2	1:C:188:ARG:CZ	2.95	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:B:378:PHE:HE1	1:B:461:ILE:HD13	1.82	0.43
1:C:868:SER:HA	1:C:871:ILE:HG12	1.99	0.43
1:C:701:ALA:O	1:C:705:ARG:HG3	2.18	0.43
1:C:380:LYS:HE3	1:C:435:ASP:OD1	2.18	0.43
1:B:684:TYR:C	1:B:684:TYR:CD1	2.92	0.43
1:C:810:ASN:CB	1:C:813:LYS:HD3	2.49	0.43
1:B:888:LEU:HD21	1:B:915:ILE:CG2	2.49	0.43
1:B:449:ARG:O	1:B:449:ARG:HG2	2.19	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: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:C:782:TRP:CE2	1:C:805:LEU:HD22	2.54	0.42
1:A:78:GLY:HA3	1:A:151:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:GLN:HE21	1:C:745:GLN:NE2	2.17	0.42
1:B:792:SER:OG	1:B:793:LEU:N	2.51	0.42
1:A:590:ILE:HG13	1:B:470:TYR:CD1	2.53	0.42
1:C:620:LEU:HD13	1:C:639:LEU:HD21	2.01	0.42
1:B:888:LEU:HD21	1:B:915:ILE:HG22	2.01	0.42
1:A:810:ASN:ND2	1:A:813:LYS:HG3	2.34	0.42
1:A:293:TYR:CE2	1:A:382:MET:HG3	2.52	0.42
1:C:850:TRP:CE3	1:C:850:TRP:HA	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:C:373:TRP:HA	1:C:438:TYR:CD2	2.54	0.42
1:A:815:GLN:HA	1:A:818:LEU:HD12	2.02	0.42
1:B:177:LEU:HD13	1:B:254:PHE:CZ	2.54	0.42
1:B:408:MET:CE	1:B:609:ILE:HG23	2.49	0.42
1:A:261:THR:CG2	1:A:265:VAL:H	2.29	0.42
1:C:543:HIS:NE2	1:C:586:THR:OG1	2.42	0.42
1:A:411:ASP:CG	1:A:529:GLY:HA2	2.39	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:A:885:ARG:O	1:A:888:LEU:HB2	2.20	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: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:595:VAL:HG12	1:A:596:GLU:N	2.34	0.42
1:A:311:ILE:HB	1:A:314:PHE:HB2	2.00	0.42
1:A:473:THR:HG22	1:A:474:LYS:N	2.33	0.42
1:A:343:SER:O	1:A:347:ILE:HG23	2.19	0.42
1:C:128:GLN:O	1:C:130:GLN:HG3	2.20	0.42
1:B:702:PHE:CE1	1:B:932:TRP:HZ3	2.38	0.42
4:C:5002:NAG:O7	4:C:5005:MAN:H62	2.20	0.42
1:B:314:PHE:CE2	1:B:317:GLY:C	2.93	0.42
1:A:621:THR:HG22	1:A:660:LEU:CD2	2.49	0.42
1:C:888:LEU:O	1:C:892:LYS:HG3	2.20	0.42
1:A:183:GLU:HA	1:A:184:PRO:HA	1.82	0.42
1:C:732:LEU:CD1	1:C:767:VAL:HG12	2.49	0.42
1:C:556:ALA:N	1:C:557:PRO:CD	2.82	0.42
1:A:457:PHE:CD1	1:A:482:MET:CE	3.03	0.42
1:C:473:THR:CG2	1:C:474:LYS:N	2.82	0.42
1:A:520:MET:HA	1:A:564:HIS:HB2	2.01	0.42
1:A:207:ILE:HG12	1:A:236:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:PHE:O	1:B:385:VAL:C	2.57	0.42
1:C:125:HIS:HD2	1:C:128:GLN:H	1.66	0.42
1:C:613:GLU:HG3	1:C:614:ASP:H	1.85	0.42
1:A:125:HIS:CE1	1:A:128:GLN:NE2	2.88	0.42
1:B:556:ALA:N	1:B:557:PRO:CD	2.82	0.42
1:A:872:ALA:O	1:A:875:VAL:CG1	2.61	0.42
1:A:367:GLU:OE1	1:A:474:LYS:CE	2.63	0.42
1:C:464:TYR:CE1	1:C:473:THR:HG21	2.55	0.42
1:B:90:THR:O	1:B:139:LEU:HG	2.20	0.42
1:C:850:TRP:HE3	1:C:850:TRP:HA	1.84	0.42
1:A:366:MET:HG3	1:A:368:TRP:O	2.19	0.42
1:B:599:LYS:HE2	1:B:639:LEU:HG	2.00	0.42
1:B:181:GLN:NE2	3:B:1001:BES:H9	2.35	0.42
1:A:702:PHE:CZ	1:A:932:TRP:CH2	3.08	0.42
1:A:379:ALA:O	1:A:383:GLU:HG3	2.20	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:C:378:PHE:CZ	1:C:382:MET:CE	3.03	0.42
1:A:850:TRP:HE3	1:A:850:TRP:HA	1.85	0.42
1:A:168:ARG:HA	1:A:173:GLU:O	2.20	0.42
1:A:544:MET:HE2	1:A:567:LEU:CD1	2.50	0.41
1:A:314:PHE:HE2	1:A:317:GLY:C	2.24	0.41
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:C:698:GLN:HE21	1:C:698:GLN:HB3	1.70	0.41
1:C:366:MET:HG3	1:C:368:TRP:O	2.20	0.41
1:B:562:LEU:HD22	1:B:562:LEU:HA	1.92	0.41
1:C:478:LEU:HD13	1:C:479:TRP:CZ3	2.55	0.41
1:A:792:SER:O	1:A:793:LEU:HB2	2.20	0.41
1:A:186:ALA:O	1:A:189:MET:HB2	2.19	0.41
1:C:754:TRP:CD1	1:C:763:LEU:HD11	2.55	0.41
1:B:520:MET:HG3	1:B:564:HIS:HB2	2.03	0.41
1:A:603:GLY:O	1:A:604:MET:HB3	2.20	0.41
1:B:440:LYS:O	1:B:444:ILE:HG12	2.20	0.41
1:C:411:ASP:OD1	1:C:529:GLY:N	2.53	0.41
1:A:411:ASP:OD1	1:A:529:GLY:N	2.51	0.41
1:A:752:ARG:HB2	1:A:752:ARG:HE	1.60	0.41
1:A:842:ASN:HA	1:A:843:PRO:HD2	1.92	0.41
1:B:733:LEU:O	1:B:737:VAL:HG23	2.19	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.90	0.41
1:C:322:TRP:CZ2	1:C:363:LEU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:THR:CG2	1:B:391:HIS:CD2	3.02	0.41
1:B:100:LEU:HD22	1:B:151:TYR:CD2	2.56	0.41
1:B:183:GLU:HA	1:B:184:PRO:HA	1.78	0.41
1:A:807:ARG:NH1	1:A:843:PRO:HD2	2.35	0.41
1:C:185:THR:HG23	1:C:188:ARG:NH2	2.35	0.41
1:A:67:ILE:CD1	1:A:249:PHE:CE1	3.03	0.41
1:B:97:SER:HB3	1:B:131:ILE:HD11	2.01	0.41
1:A:229:GLU:OE1	4:A:5004:MAN:O2	2.39	0.41
1:B:850:TRP:CE3	1:B:850:TRP:HA	2.56	0.41
1:A:807:ARG:HH12	1:A:843:PRO:HD2	1.84	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:B:97:SER:HB3	1:B:131:ILE:CG1	2.51	0.41
1:A:884:THR:HG22	1:A:886:THR:H	1.86	0.41
1:A:764:PRO:O	1:A:767:VAL:HG22	2.20	0.41
1:B:451:TYR:CD2	1:B:452:LEU:HD12	2.51	0.41
1:B:228:ALA:HB3	1:B:231:LEU:HB2	2.02	0.41
1:B:850:TRP:HE3	1:B:850:TRP:HA	1.85	0.41
1:A:884:THR:HB	1:A:887:ARG:HB2	2.02	0.41
1:A:242:MET:HB3	1:A:322:TRP:CZ3	2.55	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:C:183:GLU:HA	1:C:184:PRO:HA	1.85	0.41
1:B:624:LEU:HD12	1:B:660:LEU:HD21	2.03	0.41
1:B:810:ASN:HB2	1:B:813:LYS:HD2	2.03	0.41
1:B:520:MET:HG3	1:B:564:HIS:CB	2.51	0.41
1:B:368:TRP:CG	1:B:369:TRP:N	2.89	0.41
1:C:731:LEU:HD23	1:C:731:LEU:HA	1.75	0.41
1:B:699:PHE:HE2	1:B:703:LEU:HD11	1.86	0.41
1:C:328:ARG:CZ	1:C:331:ALA:HB2	2.51	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:A:320:GLU:N	1:A:320:GLU:OE1	2.46	0.41
1:A:319:MET:HE1	1:A:320:GLU:OE2	2.21	0.41
1:A:162:PHE:CD1	1:A:249:PHE:HE1	2.39	0.41
1:A:850:TRP:CE3	1:A:850:TRP:HA	2.55	0.41
1:B:851:GLN:O	1:B:855:LYS:HG3	2.20	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:B:764:PRO:HB2	1:B:767:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:HE1	1:A:238:VAL:HG13	1.86	0.41
1:B:681:ILE:N	1:B:682:PRO:CD	2.84	0.41
1:C:548:HIS:ND1	1:C:559:THR:HG21	2.36	0.41
1:A:301:TYR:HA	1:A:302:PRO:HD3	1.86	0.41
1:B:533:ILE:HD11	1:B:565:VAL:HG11	2.03	0.40
1:C:908:VAL:HG13	1:C:911:THR:OG1	2.21	0.40
1:B:810:ASN:CG	1:B:813:LYS:HD2	2.42	0.40
1:B:331:ALA:HA	1:B:347:ILE:HG22	2.03	0.40
1:B:815:GLN:O	1:B:818:LEU:HB2	2.20	0.40
1:A:556:ALA:N	1:A:557:PRO:CD	2.84	0.40
1:A:758:ASN:C	1:A:760:ASN:N	2.73	0.40
1:C:125:HIS:CD2	1:C:128:GLN:HG3	2.57	0.40
1:A:177:LEU:HD13	1:A:254:PHE:HZ	1.86	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:556:ALA:HB3	1:B:557:PRO:HD3	2.02	0.40
1:A:310:ALA:HB2	1:A:332:LEU:HD23	2.03	0.40
1:C:337:GLU:HG3	1:C:337:GLU:O	2.21	0.40
1:B:114:ARG:CA	1:B:117:GLU:HG3	2.49	0.40
1:C:96:HIS:CD2	1:C:195:ASP:HB3	2.56	0.40
1:B:603:GLY:O	1:B:604:MET:HB3	2.20	0.40
1:C:357:HIS:CE1	1:C:375:ASN:ND2	2.89	0.40
1:C:183:GLU:OE1	3:C:1001:BES:N2	2.55	0.40
1:A:595:VAL:HG12	1:A:597:TRP:N	2.36	0.40
1:A:449:ARG:HG3	1:A:457:PHE:CG	2.56	0.40
1:C:911:THR:O	1:C:915:ILE:HG13	2.21	0.40
1:C:261:THR:CG2	1:C:265:VAL:HB	2.51	0.40
1:A:139:LEU:HB3	1:A:145:TYR:HE1	1.87	0.40
1:B:277:ASN:HD22	1:B:277:ASN:N	2.19	0.40
1:A:196:GLU:HB2	1:A:199:PHE:HD2	1.86	0.40
1:C:167:TYR:CE1	1:C:175:ARG:HB2	2.57	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%)	34	74
1	B	809/921 (88%)	755 (93%)	52 (6%)	2 (0%)	52	86
1	C	805/921 (87%)	753 (94%)	51 (6%)	1 (0%)	56	89
All	All	2418/2763 (88%)	2258 (93%)	153 (6%)	7 (0%)	46	81

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	733/819 (90%)	710 (97%)	23 (3%)	47	81
1	B	734/819 (90%)	711 (97%)	23 (3%)	47	81
1	C	734/819 (90%)	711 (97%)	23 (3%)	47	81
All	All	2201/2457 (90%)	2132 (97%)	69 (3%)	47	81

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
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

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Mol	Chain	Res	Type
1	B	885	ARG
1	B	914	THR
1	B	924	LYS
1	B	934	GLN
1	C	95	LEU
1	C	175	ARG
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

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Mol	Chain	Res	Type
1	A	634	ASN
1	A	641	ASN
1	A	645	GLN
1	A	698	GLN
1	A	745	GLN
1	A	830	GLN
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 (i)

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

5.5 Carbohydrates (i)

12 carbohydrates are modelled in this entry.

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	$\#\|Z\|>2$
4	NAG	A	5001	1,4	14,14,15	0.83	0	15,19,21	2.12	5 (33%)
4	NAG	A	5002	4	14,14,15	0.62	0	15,19,21	2.12	3 (20%)
4	BMA	A	5003	4	11,11,12	0.41	0	14,15,17	0.71	0
4	MAN	A	5004	4	11,11,12	0.57	0	14,15,17	0.90	0
4	MAN	A	5005	4	11,11,12	0.89	0	14,15,17	1.71	3 (21%)
6	NAG	B	5001	1,6	14,14,15	0.74	0	15,19,21	1.21	1 (6%)
6	NAG	B	5002	6	14,14,15	0.63	0	15,19,21	2.18	3 (20%)
4	NAG	C	5001	1,4	14,14,15	1.03	2 (14%)	15,19,21	2.15	5 (33%)
4	NAG	C	5002	4	14,14,15	0.72	0	15,19,21	2.53	4 (26%)
4	BMA	C	5003	4	11,11,12	0.38	0	14,15,17	0.68	0
4	MAN	C	5004	4	11,11,12	0.44	0	14,15,17	0.80	0
4	MAN	C	5005	4	11,11,12	0.74	0	14,15,17	1.21	2 (14%)

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
4	NAG	A	5001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	5002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	5003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5004	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5005	4	-	0/2/19/22	0/1/1/1
6	NAG	B	5001	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	5002	6	-	0/6/23/26	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	4	-	0/6/23/26	0/1/1/1
4	BMA	C	5003	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5004	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5005	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5001	NAG	C4-C3	-2.07	1.47	1.52
4	C	5001	NAG	O4-C4	-2.02	1.38	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	5002	NAG	O5-C5-C6	-6.76	92.71	107.35
4	A	5002	NAG	O5-C5-C6	-5.98	94.40	107.35
6	B	5002	NAG	O5-C5-C6	-5.91	94.55	107.35
4	C	5001	NAG	C3-C2-N2	-4.34	100.17	110.56
4	C	5001	NAG	O4-C4-C3	-4.26	100.75	110.34
4	C	5002	NAG	C1-O5-C5	-3.66	107.60	112.25
6	B	5002	NAG	C4-C3-C2	-3.47	105.84	111.23
4	C	5002	NAG	C4-C3-C2	-3.44	105.88	111.23
4	A	5001	NAG	O3-C3-C4	-3.44	102.59	110.34
4	A	5001	NAG	C3-C4-C5	-3.32	104.41	110.20
4	A	5001	NAG	O4-C4-C3	-3.28	102.96	110.34
4	A	5005	MAN	C6-C5-C4	-3.23	105.05	113.02
4	A	5001	NAG	O3-C3-C2	-3.15	102.88	109.11
4	A	5002	NAG	C4-C3-C2	-2.87	106.77	111.23
4	A	5001	NAG	C3-C2-N2	-2.76	103.96	110.56
4	C	5001	NAG	C3-C4-C5	-2.57	105.72	110.20
4	C	5001	NAG	O3-C3-C4	-2.20	105.39	110.34
4	C	5005	MAN	C6-C5-C4	-2.17	107.66	113.02
4	A	5005	MAN	O3-C3-C4	-2.15	105.49	110.34
4	C	5001	NAG	O3-C3-C2	-2.14	104.87	109.11
4	C	5005	MAN	O5-C5-C6	2.81	113.42	107.35
6	B	5001	NAG	C1-O5-C5	2.95	115.99	112.25
4	A	5005	MAN	O5-C5-C6	3.40	114.70	107.35
4	A	5002	NAG	C6-C5-C4	3.84	122.48	113.02
6	B	5002	NAG	C6-C5-C4	3.93	122.70	113.02
4	C	5002	NAG	C6-C5-C4	4.02	122.93	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	5001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5001	NAG	3	0
4	A	5004	MAN	1	0
6	B	5001	NAG	1	0
4	C	5002	NAG	1	0
4	C	5005	MAN	1	0

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	0.50	0	19,29,29	0.82	1 (5%)
5	NAG	A	6000	1	14,14,15	0.89	1 (7%)	15,19,21	1.37	1 (6%)
5	NAG	A	6001	1	14,14,15	1.26	2 (14%)	15,19,21	1.38	3 (20%)
3	BES	B	1001	2	19,22,22	0.52	0	19,29,29	0.88	1 (5%)
5	NAG	B	6000	1	14,14,15	0.63	0	15,19,21	1.03	1 (6%)
3	BES	C	1001	2	19,22,22	0.44	0	19,29,29	0.96	1 (5%)

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
5	NAG	A	6000	1	-	0/6/23/26	0/1/1/1
5	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
5	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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6000	NAG	O5-C1	2.22	1.47	1.43
5	A	6001	NAG	O5-C1	2.61	1.48	1.43
5	A	6001	NAG	C1-C2	3.20	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1001	BES	C4-N1-C3	-2.92	118.88	123.43
5	A	6001	NAG	C6-C5-C4	-2.74	106.26	113.02
3	B	1001	BES	C4-N1-C3	-2.41	119.67	123.43
3	A	1001	BES	C7-C6-C1	-2.07	109.17	113.53
5	A	6001	NAG	C4-C3-C2	-2.03	108.08	111.23
5	B	6000	NAG	C1-O5-C5	2.16	114.99	112.25
5	A	6001	NAG	C1-O5-C5	2.88	115.90	112.25
5	A	6000	NAG	C1-O5-C5	3.63	116.85	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	6001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.22	23 (2%)	56	36	26, 57, 133, 238	11 (1%)
1	B	821/921 (89%)	-0.14	36 (4%)	38	22	24, 57, 130, 223	11 (1%)
1	C	818/921 (88%)	-0.24	28 (3%)	49	30	28, 57, 130, 223	12 (1%)
All	All	2457/2763 (88%)	-0.20	87 (3%)	48	29	24, 57, 131, 238	34 (1%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	SER	9.9
1	B	558	ASP	9.0
1	B	557	PRO	8.6
1	B	794	SER	8.6
1	B	825	ASP	7.6
1	B	339	SER	7.6
1	B	827	ILE	7.6
1	B	826	LYS	7.3
1	A	829	THR	6.1
1	C	794	SER	5.8
1	B	829	THR	5.7
1	B	792	SER	4.8
1	C	907	CYS	4.8
1	C	791	PHE	4.7
1	B	911	THR	4.6
1	C	793	LEU	4.6
1	A	889	GLU	4.4
1	B	556	ALA	4.4
1	A	857	TRP	4.3
1	C	762	SER	4.3
1	C	792	SER	4.3
1	B	824	GLY	4.3
1	A	339	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	757	SER	4.2
1	C	558	ASP	4.0
1	B	338	LYS	3.9
1	B	790	GLN	3.9
1	B	791	PHE	3.9
1	B	908	VAL	3.7
1	C	908	VAL	3.7
1	C	789	TYR	3.6
1	C	824	GLY	3.6
1	B	862	GLN	3.6
1	A	907	CYS	3.5
1	B	828	LYS	3.5
1	C	829	THR	3.4
1	A	794	SER	3.3
1	A	832	PHE	3.3
1	B	912	ILE	3.3
1	C	869	SER	3.3
1	B	337	GLU	3.1
1	B	759	GLY	3.1
1	A	871	ILE	3.0
1	A	851	GLN	2.9
1	A	415	SER	2.9
1	B	855	LYS	2.8
1	C	110	GLY	2.7
1	C	825	ASP	2.7
1	A	862	GLN	2.6
1	B	858	ASN	2.6
1	B	784	PHE	2.5
1	B	891	VAL	2.5
1	B	613	GLU	2.4
1	A	892	LYS	2.4
1	A	827	ILE	2.4
1	B	336	ALA	2.4
1	A	888	LEU	2.4
1	B	863	LYS	2.4
1	C	760	ASN	2.4
1	C	858	ASN	2.4
1	B	798	LYS	2.4
1	C	830	GLN	2.3
1	B	485	ILE	2.3
1	C	860	LEU	2.3
1	C	892	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	558	ASP	2.3
1	C	485	ILE	2.3
1	C	909	GLN	2.3
1	C	857	TRP	2.3
1	B	140	LEU	2.3
1	B	755	LYS	2.3
1	B	415	SER	2.3
1	A	890	GLU	2.3
1	B	871	ILE	2.2
1	B	868	SER	2.2
1	C	415	SER	2.2
1	C	850	TRP	2.2
1	A	362	ASN	2.2
1	C	911	THR	2.1
1	A	789	TYR	2.1
1	A	752	ARG	2.1
1	A	342	SER	2.1
1	B	316	SER	2.1
1	A	831	GLU	2.0
1	A	551	LYS	2.0
1	C	826	LYS	2.0
1	A	483	ALA	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)

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, 95^{th} 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
4	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
6	NAG	B	5001	14/15	0.91	0.21	1.00	50,93,110,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	B	5002	14/15	0.75	0.25	-	118,161,189,212	0
4	BMA	C	5003	11/12	0.85	0.26	-	43,135,191,223	0
4	MAN	A	5004	11/12	0.56	0.34	-	111,168,187,189	0
4	NAG	C	5002	14/15	0.86	0.34	-	47,135,257,284	0
4	NAG	A	5002	14/15	0.88	0.18	-	60,85,108,108	0
4	BMA	A	5003	11/12	0.89	0.17	-	51,86,129,131	0
4	MAN	A	5005	11/12	0.83	0.30	-	33,95,172,209	0
4	MAN	C	5005	11/12	0.81	0.35	-	86,142,212,223	0

6.4 Ligands

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, 95^{th} 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
3	BES	B	1001	22/22	0.88	0.38	3.50	121,167,185,218	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
5	NAG	A	6000	14/15	0.82	0.19	-	76,119,141,145	0
5	NAG	A	6001	14/15	0.74	0.17	-	72,140,150,153	0
5	NAG	B	6000	14/15	0.74	0.28	-	59,128,146,153	0

6.5 Other polymers

There are no such residues in this entry.