



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:01 PM GMT

PDB ID : 3SE6  
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2  
Authors : Birtley, J.R.; Saridakis, E.; Stratikos, E; Mavridis, I.M.  
Deposited on : 2011-06-10  
Resolution : 3.08 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 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

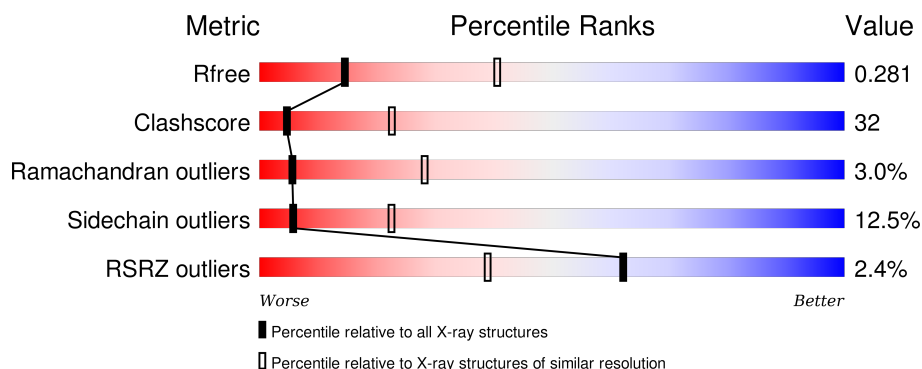
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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  $\geq 3$ , 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	967	<div> <div></div> <div>43%</div> <div>39%</div> <div>8%</div> <div>10%</div> </div>
1	B	967	<div> <div>3%</div> <div>39%</div> <div>41%</div> <div>8%</div> <div>11%</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
4	NAG	A	1073	-	-	-	X
5	NAG	A	1075	-	-	-	X
5	NAG	B	1081	-	-	-	X
7	MAN	B	1079	X	-	-	-
7	MAN	B	1080	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14348 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	2	2	0
			7050	4548	1173	1302	27			
1	B	859	Total	C	N	O	S	0	0	0
			6978	4504	1160	1287	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	ENGINEERED MUTATION	UNP Q6P179
A	392	ASN	LYS	SEE REMARK 999	UNP Q6P179
A	961	ARG	-	EXPRESSION TAG	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG	UNP Q6P179
A	967	HIS	-	EXPRESSION TAG	UNP Q6P179
B	2	VAL	PHE	ENGINEERED MUTATION	UNP Q6P179
B	392	ASN	LYS	SEE REMARK 999	UNP Q6P179
B	961	ARG	-	EXPRESSION TAG	UNP Q6P179
B	962	HIS	-	EXPRESSION TAG	UNP Q6P179
B	963	HIS	-	EXPRESSION TAG	UNP Q6P179
B	964	HIS	-	EXPRESSION TAG	UNP Q6P179
B	965	HIS	-	EXPRESSION TAG	UNP Q6P179
B	966	HIS	-	EXPRESSION TAG	UNP Q6P179
B	967	HIS	-	EXPRESSION TAG	UNP Q6P179

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

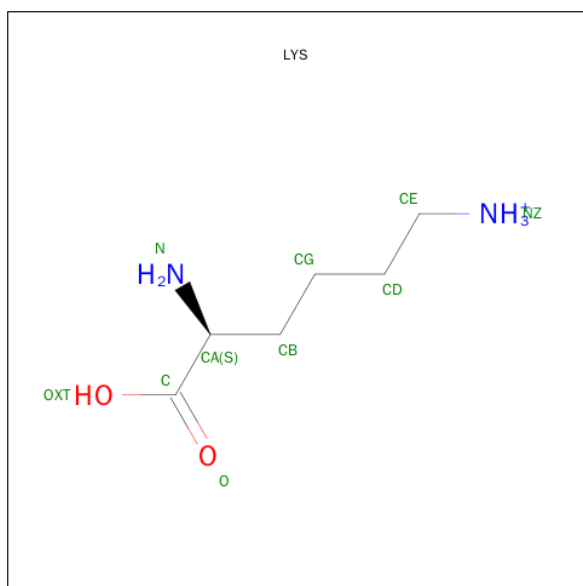
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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

- Molecule 3 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).

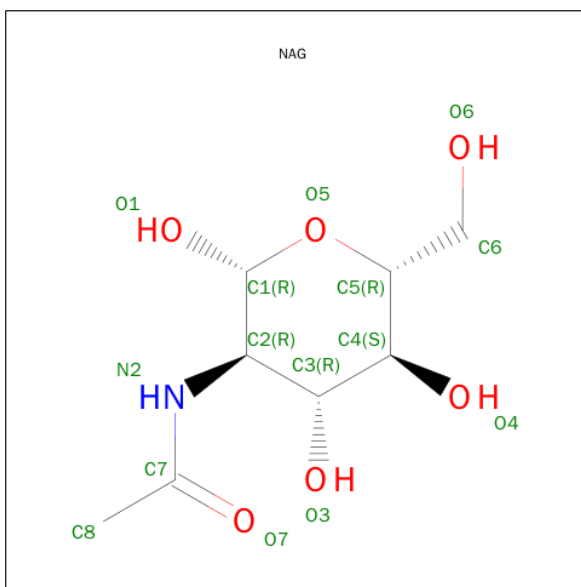


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

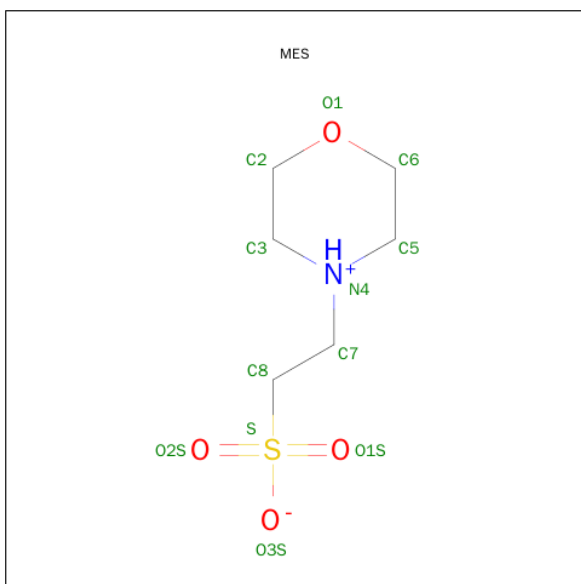
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	53	Total	O	0	0
			53	53		







1955	1956	1961	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.58Å 134.36Å 128.01Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	11.00 – 3.08 20.03 – 3.08	Depositor EDS
% Data completeness (in resolution range)	94.3 (11.00-3.08) 93.3 (20.03-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.212 , 0.277 0.214 , 0.281	Depositor DCC
$R_{free}$ test set	2194 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 70.6	EDS
Estimated twinning fraction	0.018 for -h,-l,-k 0.005 for -h,l,k 0.034 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46141 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG, MES, 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	0.40	0/7227	0.58	1/9794 (0.0%)
1	B	0.41	0/7148	0.58	0/9686
All	All	0.41	0/14375	0.58	1/19480 (0.0%)

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
7	B	2	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	923	ALA	N-CA-C	-5.60	95.88	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1079	MAN	C1
7	B	1080	MAN	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	7050	0	6987	431	0
1	B	6978	0	6946	474	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	12	1	0
3	B	10	0	12	2	0
4	A	56	0	50	5	0
5	A	28	0	26	0	0
5	B	14	0	13	3	0
6	A	12	0	12	2	0
6	B	12	0	12	4	0
7	B	50	0	43	1	0
8	A	73	0	0	4	0
8	B	53	0	0	12	0
All	All	14348	0	14113	904	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 32.

All (904) 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:B:56:ALA:HB1	1:B:61:ARG:HA	1.23	1.09
1:A:56:ALA:HB1	1:A:57:THR:HA	1.34	1.06
1:B:245:GLU:HG2	1:B:246:GLY:H	1.27	0.98
1:A:245:GLU:HG2	1:A:246:GLY:H	1.23	0.98
1:A:544:GLN:HE21	1:A:584:TYR:HD1	1.16	0.93
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.32	0.93
1:A:533:GLU:HG2	1:A:533:GLU:O	1.70	0.92
1:B:544:GLN:HE21	1:B:584:TYR:HD1	1.16	0.92
1:B:386:TRP:CD1	1:B:446:ILE:HD13	2.06	0.90
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.52	0.89
1:B:56:ALA:HB1	1:B:61:ARG:CA	2.05	0.86
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.57	0.85
1:B:138:LYS:HB3	1:B:151:LEU:HB2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:HG3	1:A:211:PHE:CD1	2.11	0.85
1:A:626:ASP:HA	1:A:657:LYS:HB2	1.58	0.85
1:A:465:LEU:HD13	1:A:538:MET:SD	2.17	0.84
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.59	0.84
1:B:75:PRO:HG3	1:B:211:PHE:CD1	2.12	0.84
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.11	0.84
1:B:666:VAL:HG21	1:B:683:MET:SD	2.19	0.82
1:B:152:VAL:HG21	1:B:156:LEU:HD21	1.60	0.82
1:A:73:VAL:HG11	1:A:108:ILE:HG12	1.61	0.82
1:A:677:LEU:HG	1:A:681:LEU:HD23	1.61	0.82
1:B:135:LYS:HE2	1:B:153:PRO:HG2	1.62	0.82
1:A:56:ALA:CB	1:A:57:THR:HA	2.10	0.82
1:B:677:LEU:HG	1:B:681:LEU:HD23	1.61	0.82
1:A:384:GLU:HA	1:A:489:ASN:HD22	1.45	0.81
1:B:817:SER:O	1:B:821:GLN:HG3	1.81	0.81
1:A:135:LYS:HE2	1:A:153:PRO:HG2	1.63	0.81
1:B:73:VAL:HG11	1:B:108:ILE:HG12	1.61	0.81
1:B:801:THR:HG23	1:B:804:GLY:H	1.46	0.80
1:B:258:LYS:HG2	5:B:1081:NAG:H62	1.61	0.80
1:A:152:VAL:HG21	1:A:156:LEU:HD21	1.64	0.80
1:A:801:THR:HG23	1:A:804:GLY:H	1.46	0.80
1:A:604:ILE:HD12	1:A:604:ILE:H	1.47	0.79
1:A:877:ARG:HG3	1:A:917:PHE:CD1	2.17	0.79
1:A:125:GLU:OE1	1:A:125:GLU:HA	1.80	0.79
1:A:666:VAL:HG21	1:A:683:MET:SD	2.23	0.79
1:B:604:ILE:H	1:B:604:ILE:HD12	1.46	0.79
1:B:465:LEU:HD13	1:B:538:MET:SD	2.23	0.79
1:B:877:ARG:HG3	1:B:917:PHE:CD1	2.17	0.79
1:A:741:ASP:OD2	1:A:787:PRO:HB3	1.82	0.78
1:A:416:TYR:HD2	1:A:416:TYR:C	1.88	0.77
1:B:56:ALA:CB	1:B:61:ARG:HA	2.11	0.76
1:A:817:SER:O	1:A:821:GLN:HG3	1.85	0.76
1:B:416:TYR:C	1:B:416:TYR:HD2	1.89	0.76
1:A:662:LEU:O	1:A:666:VAL:HG23	1.85	0.76
1:B:551:VAL:HG12	1:B:634:HIS:HB3	1.66	0.75
1:B:741:ASP:OD2	1:B:787:PRO:HB3	1.85	0.75
1:B:412:GLN:OE1	1:B:746:TRP:HD1	1.70	0.75
1:A:245:GLU:HG2	1:A:246:GLY:N	2.02	0.75
1:A:85:ASN:HB3	1:A:88:SER:HB3	1.68	0.75
1:A:364:VAL:O	1:A:368:ILE:HG13	1.87	0.75
1:B:421:CYS:O	1:B:424:VAL:HG12	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASN:HB3	1:B:88:SER:HB3	1.70	0.74
4:A:1073:NAG:H62	4:A:1074:NAG:O5	1.88	0.74
1:A:421:CYS:O	1:A:424:VAL:HG12	1.88	0.74
1:B:364:VAL:O	1:B:368:ILE:HG13	1.88	0.73
1:B:286:ILE:HG21	1:B:296:THR:HB	1.69	0.73
1:B:838:LEU:HD23	1:B:871:LEU:HD21	1.70	0.73
1:B:544:GLN:NE2	1:B:584:TYR:HD1	1.85	0.73
1:A:551:VAL:HG12	1:A:634:HIS:HB3	1.70	0.73
1:B:662:LEU:O	1:B:666:VAL:HG23	1.89	0.73
1:A:838:LEU:HD23	1:A:871:LEU:HD21	1.69	0.73
1:A:412:GLN:OE1	1:A:746:TRP:HD1	1.72	0.73
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.71	0.72
1:A:544:GLN:NE2	1:A:584:TYR:HD1	1.85	0.72
1:A:286:ILE:HG21	1:A:296:THR:HB	1.72	0.72
1:B:385:TRP:CD1	8:B:1013:HOH:O	2.42	0.71
1:A:442:THR:HG23	1:A:445:GLN:HG3	1.73	0.71
1:B:537:MET:O	1:B:540:THR:HG23	1.90	0.71
1:A:727:LEU:HD21	1:A:761:LEU:HB3	1.72	0.71
1:A:416:TYR:C	1:A:416:TYR:CD2	2.62	0.71
1:B:236:MET:CE	1:B:256:THR:HA	2.21	0.70
1:B:590:LEU:HG	8:B:1014:HOH:O	1.91	0.70
1:B:710:MET:HB3	1:B:719:SER:HB3	1.74	0.70
1:B:731:LYS:HE3	1:B:763:HIS:CE1	2.26	0.70
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.73	0.70
1:B:832:LYS:HB3	1:B:867:LYS:HE3	1.72	0.70
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.73	0.70
1:B:319:PRO:HB2	1:B:320:LEU:HD23	1.72	0.70
1:A:416:TYR:CE2	1:A:419:ASN:HB2	2.27	0.70
1:A:537:MET:O	1:A:540:THR:HG23	1.91	0.70
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.72	0.70
1:B:385:TRP:C	8:B:1013:HOH:O	2.29	0.69
1:B:239:VAL:HG12	1:B:240:LYS:HE3	1.74	0.69
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.75	0.69
1:B:634:HIS:HE1	1:B:675:LEU:HD13	1.57	0.69
1:B:604:ILE:HD12	1:B:604:ILE:N	2.07	0.69
1:B:416:TYR:CE2	1:B:419:ASN:HB2	2.27	0.69
1:A:832:LYS:HB3	1:A:867:LYS:HE3	1.75	0.69
1:B:58:ASN:N	1:B:58:ASN:HD22	1.91	0.68
1:B:697:LEU:CD1	1:B:750:LEU:HD13	2.23	0.68
1:A:416:TYR:HD2	1:A:416:TYR:O	1.77	0.68
1:B:90:ASP:HB3	1:B:171:LYS:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:HIS:HE1	1:A:675:LEU:HD13	1.59	0.68
1:B:488:ARG:HG2	1:B:489:ASN:H	1.59	0.68
1:A:565:ARG:HD2	1:A:584:TYR:CE2	2.29	0.67
1:B:236:MET:HE3	1:B:256:THR:HA	1.75	0.67
1:A:710:MET:HB3	1:A:719:SER:HB3	1.77	0.67
1:A:272:HIS:CE1	1:A:290:PRO:HB3	2.29	0.67
1:B:245:GLU:HG2	1:B:246:GLY:N	2.05	0.67
1:A:565:ARG:HD3	1:A:581:GLN:N	2.10	0.67
1:B:812:TYR:CE1	1:B:821:GLN:HB3	2.30	0.67
1:B:915:LYS:O	1:B:919:GLU:HG2	1.93	0.67
1:B:135:LYS:HE2	1:B:153:PRO:CG	2.24	0.67
1:B:924:GLN:O	1:B:926:SER:N	2.27	0.67
1:B:398:TYR:OH	1:B:402:ILE:HD11	1.95	0.67
1:A:528:LEU:HB3	1:A:529:GLY:HA2	1.76	0.67
1:A:727:LEU:HD11	1:A:763:HIS:HB2	1.77	0.67
1:A:278:THR:HG23	1:A:282:VAL:H	1.59	0.67
1:A:697:LEU:CD1	1:A:750:LEU:HD13	2.25	0.67
1:A:442:THR:CG2	1:A:445:GLN:HG3	2.26	0.66
1:A:90:ASP:HB3	1:A:171:LYS:HA	1.76	0.66
1:B:681:LEU:HB3	1:B:955:TRP:CE2	2.30	0.66
1:B:727:LEU:HD21	1:B:761:LEU:HB3	1.76	0.66
1:B:58:ASN:ND2	1:B:58:ASN:N	2.42	0.66
1:A:488:ARG:HG2	1:A:489:ASN:H	1.60	0.66
1:A:604:ILE:HD12	1:A:604:ILE:N	2.10	0.66
1:B:272:HIS:CE1	1:B:290:PRO:HB3	2.31	0.66
1:A:398:TYR:OH	1:A:402:ILE:HD11	1.94	0.66
1:A:236:MET:CE	1:A:256:THR:HA	2.25	0.66
1:B:338:ASN:HB2	1:B:341:LEU:O	1.96	0.66
1:A:566:PHE:CE2	1:A:632:ILE:HD12	2.30	0.65
1:A:338:ASN:HB2	1:A:341:LEU:O	1.96	0.65
1:B:416:TYR:HD2	1:B:416:TYR:O	1.80	0.65
1:B:330:ASP:OD1	1:B:851:LYS:HD2	1.96	0.65
1:B:58:ASN:H	1:B:58:ASN:HD22	1.45	0.65
1:B:313:TYR:HE2	1:B:478:ILE:HD11	1.62	0.65
1:A:915:LYS:O	1:A:919:GLU:HG2	1.94	0.65
1:A:135:LYS:HE2	1:A:153:PRO:CG	2.26	0.64
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.32	0.64
1:B:416:TYR:CD2	1:B:416:TYR:C	2.63	0.64
1:A:236:MET:HE3	1:A:256:THR:HA	1.79	0.64
1:A:141:SER:HA	1:A:148:ILE:HG22	1.80	0.64
1:B:918:PHE:CE2	1:B:934:VAL:HG11	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:GLN:NE2	8:A:1024:HOH:O	2.29	0.64
1:A:565:ARG:HH11	1:A:581:GLN:HB2	1.62	0.64
1:A:763:HIS:CD2	1:A:765:PRO:HD2	2.33	0.64
1:B:588:ILE:HD11	1:B:631:TYR:CG	2.33	0.64
1:B:777:TRP:HB2	1:B:786:ILE:CD1	2.26	0.64
1:B:141:SER:HA	1:B:148:ILE:HG22	1.80	0.63
1:A:278:THR:CG2	1:A:282:VAL:HB	2.28	0.63
1:A:697:LEU:HD13	1:A:750:LEU:HD13	1.80	0.63
1:B:214:PRO:HG3	1:B:386:TRP:CZ2	2.34	0.63
1:B:622:LYS:NZ	1:B:662:LEU:HG	2.14	0.63
1:A:533:GLU:CG	1:A:533:GLU:O	2.45	0.63
1:B:918:PHE:CE2	1:B:931:PHE:HA	2.33	0.63
1:A:56:ALA:HB1	1:A:57:THR:CA	2.22	0.63
1:A:330:ASP:OD1	1:A:851:LYS:HD2	1.98	0.63
1:B:384:GLU:HG2	1:B:489:ASN:HB3	1.81	0.63
1:B:286:ILE:CG2	1:B:296:THR:HB	2.28	0.62
1:B:727:LEU:HD11	1:B:763:HIS:HB2	1.80	0.62
1:A:582:GLU:C	1:A:583:ARG:HG2	2.20	0.62
1:A:286:ILE:CG2	1:A:296:THR:HB	2.29	0.62
1:B:605:LEU:HD12	1:B:606:LYS:N	2.15	0.62
1:B:56:ALA:HB2	1:B:62:PHE:H	1.64	0.62
1:B:566:PHE:CE2	1:B:632:ILE:HD12	2.35	0.62
1:A:830:THR:HB	1:A:865:ARG:HH21	1.64	0.62
1:B:278:THR:HG23	1:B:282:VAL:H	1.64	0.62
1:B:323:LEU:HD12	1:B:324:ASP:H	1.64	0.62
1:A:538:MET:O	1:A:542:THR:HG23	1.98	0.62
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.34	0.62
1:A:934:VAL:O	1:A:938:ILE:HG13	2.00	0.62
1:A:615:PRO:O	1:A:616:GLU:HB2	1.99	0.62
1:A:713:ARG:HB3	1:A:715:ILE:HG13	1.82	0.62
1:B:805:TRP:HH2	1:B:839:LYS:HD3	1.64	0.62
1:B:713:ARG:HB3	1:B:715:ILE:HG13	1.81	0.61
1:B:58:ASN:HA	1:B:59:GLY:C	2.21	0.61
1:A:528:LEU:HB3	1:A:529:GLY:CA	2.29	0.61
1:A:918:PHE:CE2	1:A:931:PHE:HA	2.34	0.61
1:A:433:SER:O	1:A:545:LYS:HD3	2.00	0.61
1:A:548:PRO:HG3	1:A:586:TRP:CD2	2.36	0.61
1:A:918:PHE:CE2	1:A:934:VAL:HG11	2.36	0.61
1:B:615:PRO:O	1:B:616:GLU:HB2	2.00	0.61
1:B:67:LEU:HA	1:B:145:HIS:HD2	1.64	0.61
1:A:790:VAL:O	1:A:794:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TYR:CZ	1:A:402:ILE:HD11	2.35	0.61
1:A:622:LYS:NZ	1:A:662:LEU:HG	2.15	0.61
1:A:588:ILE:HD11	1:A:631:TYR:CG	2.36	0.61
1:A:700:LEU:HD21	1:A:730:PHE:CD1	2.36	0.61
1:B:119:ASN:O	1:B:166:MET:HA	1.99	0.61
1:B:697:LEU:HD13	1:B:750:LEU:HD13	1.81	0.60
1:B:442:THR:CG2	1:B:445:GLN:HG3	2.31	0.60
1:A:605:LEU:HD12	1:A:606:LYS:N	2.16	0.60
1:B:273:SER:HA	1:B:286:ILE:O	2.01	0.60
1:B:565:ARG:HD2	1:B:584:TYR:CE2	2.37	0.60
1:A:624:ASN:OD1	1:A:627:SER:HA	2.02	0.60
1:B:538:MET:O	1:B:542:THR:HG23	2.01	0.60
1:A:67:LEU:HA	1:A:145:HIS:HD2	1.66	0.60
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.83	0.60
1:B:626:ASP:HA	1:B:657:LYS:CB	2.32	0.60
1:A:352:ASP:OD2	1:A:355:THR:HB	2.02	0.60
1:A:187:LEU:HB3	1:B:87:THR:HG22	1.84	0.60
1:B:384:GLU:HA	1:B:489:ASN:ND2	2.10	0.59
1:B:323:LEU:HD12	1:B:324:ASP:N	2.17	0.59
1:B:333:PRO:HG3	3:B:968:LYS:HE3	1.84	0.59
1:B:415:ASP:HB2	1:B:746:TRP:CZ2	2.37	0.59
1:B:86:LEU:HD21	1:B:268:VAL:HG23	1.83	0.59
1:A:239:VAL:HG12	1:A:240:LYS:HE3	1.83	0.59
1:A:313:TYR:HE2	1:A:478:ILE:HD11	1.66	0.59
1:B:934:VAL:O	1:B:938:ILE:HG13	2.03	0.59
1:A:323:LEU:HD12	1:A:324:ASP:H	1.66	0.59
1:B:906:SER:HB3	1:B:941:ASN:HB3	1.84	0.59
1:A:729:TYR:HB3	1:A:730:PHE:CD2	2.38	0.59
1:B:398:TYR:CZ	1:B:402:ILE:HD11	2.37	0.59
1:A:777:TRP:HB2	1:A:786:ILE:CD1	2.32	0.59
1:B:442:THR:HG23	1:B:445:GLN:HG3	1.83	0.59
1:A:740:SER:OG	1:A:742:LYS:HG2	2.02	0.59
1:A:278:THR:HG21	1:A:282:VAL:HB	1.85	0.58
1:B:594:THR:HG21	1:B:614:LEU:HD11	1.83	0.58
1:A:797:VAL:O	1:A:800:GLN:HG2	2.03	0.58
1:B:245:GLU:CG	1:B:246:GLY:H	2.06	0.58
1:A:582:GLU:C	1:A:583:ARG:CG	2.71	0.58
1:A:219:ASN:OD1	1:A:258:LYS:HD2	2.03	0.58
1:A:415:ASP:HB2	1:A:746:TRP:CZ2	2.38	0.58
1:A:273:SER:HA	1:A:286:ILE:O	2.03	0.58
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:HIS:O	1:B:860:HIS:HD2	1.87	0.58
1:B:813:GLU:HG2	1:B:849:VAL:HG13	1.84	0.58
1:B:729:TYR:HB3	1:B:730:PHE:CD2	2.37	0.58
1:B:540:THR:O	1:B:544:GLN:HG2	2.02	0.58
1:B:797:VAL:O	1:B:800:GLN:HG2	2.03	0.58
1:B:436:ILE:HD11	1:B:457:LYS:HG2	1.84	0.58
1:A:333:PRO:HA	6:A:1083:MES:O3S	2.04	0.58
1:B:441:GLU:HB2	1:B:445:GLN:OE1	2.04	0.58
1:B:278:THR:CG2	1:B:282:VAL:HB	2.34	0.58
1:B:624:ASN:OD1	1:B:627:SER:HA	2.04	0.58
1:B:465:LEU:HD22	1:B:496:TRP:HZ3	1.69	0.57
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.84	0.57
1:A:119:ASN:O	1:A:166:MET:HA	2.04	0.57
1:B:727:LEU:O	1:B:731:LYS:HD3	2.03	0.57
1:A:333:PRO:HB3	3:A:968:LYS:HG2	1.85	0.57
1:B:433:SER:O	1:B:545:LYS:HD3	2.04	0.57
1:B:634:HIS:HE1	1:B:675:LEU:CD1	2.17	0.57
1:A:324:ASP:C	1:A:325:LEU:HD12	2.25	0.57
1:A:540:THR:O	1:A:544:GLN:HG2	2.05	0.57
1:B:398:TYR:OH	1:B:466:LYS:HD3	2.04	0.57
1:A:158:PRO:CB	1:A:159:HIS:HD2	2.17	0.57
1:B:318:TYR:CE2	1:B:320:LEU:HB2	2.39	0.57
1:A:911:LEU:CD1	1:A:939:THR:HG22	2.34	0.57
1:A:86:LEU:HD21	1:A:268:VAL:HG23	1.85	0.57
1:B:407:THR:HG1	1:B:408:TYR:HD2	1.50	0.57
1:B:62:PHE:CD1	1:B:142:TYR:HB2	2.40	0.57
1:A:123:GLN:NE2	1:A:133:PRO:HB3	2.19	0.57
1:A:812:TYR:CE1	1:A:821:GLN:HB3	2.39	0.57
1:B:547:ILE:HG12	1:B:548:PRO:HD2	1.86	0.57
1:B:67:LEU:HB3	1:B:145:HIS:CD2	2.40	0.57
1:B:219:ASN:OD1	1:B:258:LYS:HD2	2.05	0.56
1:B:700:LEU:HD21	1:B:730:PHE:CD1	2.40	0.56
1:A:398:TYR:OH	1:A:466:LYS:HD3	2.05	0.56
1:A:925:GLY:O	1:A:926:SER:C	2.44	0.56
1:A:64:TRP:CE2	1:A:70:PRO:HG3	2.40	0.56
1:B:352:ASP:OD2	1:B:355:THR:HB	2.05	0.56
1:A:727:LEU:HD22	1:A:761:LEU:HD23	1.87	0.56
1:B:763:HIS:CD2	1:B:765:PRO:HD2	2.40	0.56
1:A:158:PRO:HB3	1:A:159:HIS:HD2	1.71	0.56
1:A:730:PHE:HD2	1:A:730:PHE:N	2.03	0.56
1:B:152:VAL:HG12	1:B:154:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:HIS:CE1	1:B:675:LEU:HD13	2.40	0.56
1:A:634:HIS:HE1	1:A:675:LEU:CD1	2.18	0.56
1:A:750:LEU:HD12	1:A:750:LEU:O	2.06	0.56
1:B:557:CYS:SG	1:B:617:LYS:HG2	2.45	0.56
1:A:813:GLU:HG2	1:A:849:VAL:HG13	1.87	0.56
1:B:72:VAL:HG13	1:B:103:ASN:HB2	1.86	0.56
1:A:245:GLU:CG	1:A:246:GLY:H	2.05	0.56
1:B:750:LEU:O	1:B:750:LEU:HD12	2.05	0.56
1:B:122:LEU:HB2	1:B:137:LEU:HD21	1.87	0.56
1:A:152:VAL:HG12	1:A:154:GLU:H	1.70	0.56
1:B:158:PRO:CB	1:B:159:HIS:HD2	2.19	0.56
1:B:80:LEU:HD22	1:B:81:PHE:N	2.21	0.56
1:A:67:LEU:HB3	1:A:145:HIS:CD2	2.42	0.55
1:A:906:SER:HB3	1:A:941:ASN:HB3	1.87	0.55
1:B:342:ILE:HD11	1:B:375:GLN:NE2	2.21	0.55
1:B:720:GLU:HA	1:B:720:GLU:OE2	2.06	0.55
1:B:696:LEU:HD23	1:B:750:LEU:HD21	1.88	0.55
1:B:796:SER:O	1:B:800:GLN:NE2	2.38	0.55
1:B:740:SER:OG	1:B:742:LYS:HG2	2.06	0.55
1:B:710:MET:O	1:B:713:ARG:O	2.25	0.55
1:B:731:LYS:HE3	1:B:763:HIS:HE1	1.70	0.55
1:A:323:LEU:HD12	1:A:324:ASP:N	2.21	0.55
1:A:214:PRO:HG3	1:A:386:TRP:CZ2	2.41	0.55
1:A:318:TYR:CE2	1:A:320:LEU:HB2	2.41	0.55
1:B:405:ASN:O	1:B:409:PRO:HG3	2.06	0.55
1:A:863:ALA:HB1	1:A:904:HIS:HE1	1.71	0.55
1:A:919:GLU:O	1:A:922:GLU:HB2	2.06	0.55
1:A:796:SER:O	1:A:800:GLN:NE2	2.39	0.55
1:A:355:THR:HG21	1:A:817:SER:OG	2.07	0.55
1:A:677:LEU:HG	1:A:681:LEU:CD2	2.34	0.55
1:A:934:VAL:CG1	1:A:935:LEU:N	2.70	0.55
1:B:830:THR:HB	1:B:865:ARG:HH21	1.71	0.55
1:A:122:LEU:HB2	1:A:137:LEU:HD21	1.88	0.55
1:B:314:PHE:O	1:B:479:ILE:HD12	2.07	0.55
1:A:655:ARG:HB2	1:A:658:ASP:HB2	1.89	0.55
1:A:626:ASP:OD1	1:A:655:ARG:HD3	2.07	0.55
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.42	0.54
1:A:860:HIS:O	1:A:860:HIS:HD2	1.90	0.54
1:B:730:PHE:N	1:B:730:PHE:HD2	2.06	0.54
1:B:588:ILE:HD11	1:B:631:TYR:CD1	2.41	0.54
1:A:731:LYS:N	1:A:732:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.41	0.54
1:A:611:THR:HG22	1:A:612:LEU:N	2.22	0.54
1:A:72:VAL:HG13	1:A:103:ASN:HB2	1.88	0.54
1:A:588:ILE:HD11	1:A:631:TYR:CD1	2.42	0.54
1:B:537:MET:CE	1:B:589:PRO:HG3	2.38	0.54
1:A:634:HIS:CE1	1:A:675:LEU:HD13	2.41	0.54
1:A:258:LYS:HG2	4:A:1073:NAG:O6	2.07	0.54
1:A:622:LYS:HZ2	1:A:662:LEU:HG	1.72	0.54
1:B:677:LEU:HG	1:B:681:LEU:CD2	2.34	0.54
1:B:730:PHE:N	1:B:730:PHE:CD2	2.76	0.54
1:B:387:ASN:CG	8:B:1013:HOH:O	2.45	0.54
1:B:697:LEU:HD11	1:B:750:LEU:HD13	1.90	0.54
1:A:720:GLU:HA	1:A:720:GLU:OE2	2.08	0.54
1:B:386:TRP:N	8:B:1013:HOH:O	2.40	0.54
1:A:855:LEU:HD22	1:A:859:LEU:HD22	1.90	0.54
1:A:416:TYR:O	1:A:418:LEU:N	2.41	0.54
1:B:718:ILE:HD12	1:B:949:LEU:HD11	1.90	0.54
1:B:257:VAL:HG23	1:B:258:LYS:O	2.08	0.54
1:B:911:LEU:CD1	1:B:939:THR:HG22	2.37	0.54
1:B:324:ASP:C	1:B:325:LEU:HD12	2.28	0.54
1:A:730:PHE:CD2	1:A:730:PHE:N	2.75	0.54
1:A:316:ILE:HD11	1:A:483:LYS:HG3	1.90	0.53
1:A:441:GLU:HB2	1:A:445:GLN:OE1	2.07	0.53
1:B:870:GLN:HE22	1:B:910:LYS:NZ	2.05	0.53
1:B:80:LEU:HD22	1:B:81:PHE:H	1.74	0.53
1:B:626:ASP:OD1	1:B:655:ARG:HD3	2.07	0.53
1:B:805:TRP:CH2	1:B:839:LYS:HD3	2.43	0.53
1:B:790:VAL:O	1:B:794:VAL:HG23	2.08	0.53
1:B:592:TYR:HA	1:B:622:LYS:O	2.09	0.53
1:B:547:ILE:HG12	1:B:548:PRO:CD	2.38	0.53
1:A:547:ILE:HG12	1:A:548:PRO:HD2	1.90	0.53
1:A:465:LEU:HD22	1:A:496:TRP:HZ3	1.74	0.53
1:A:278:THR:HG23	1:A:282:VAL:N	2.24	0.53
1:B:863:ALA:HB1	1:B:904:HIS:HE1	1.74	0.53
1:A:870:GLN:HE22	1:A:910:LYS:NZ	2.06	0.53
1:A:549:LEU:HB2	1:A:566:PHE:HD2	1.74	0.53
1:A:615:PRO:O	1:A:616:GLU:CB	2.56	0.53
1:B:278:THR:HG21	1:B:282:VAL:HB	1.89	0.53
1:B:411:LEU:HA	1:B:745:VAL:HG21	1.91	0.53
1:A:80:LEU:HD12	1:A:222:ILE:CD1	2.39	0.53
1:B:416:TYR:HE2	1:B:419:ASN:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PRO:HB3	1:B:159:HIS:HD2	1.73	0.52
1:A:696:LEU:HD23	1:A:750:LEU:HD21	1.91	0.52
1:A:190:GLU:HG2	1:B:192:ARG:HA	1.91	0.52
1:B:90:ASP:CB	1:B:171:LYS:HA	2.37	0.52
1:A:700:LEU:HD21	1:A:730:PHE:HD1	1.73	0.52
1:B:457:LYS:HE3	1:B:630:TYR:CE2	2.44	0.52
1:B:64:TRP:CE2	1:B:70:PRO:HG3	2.44	0.52
1:A:537:MET:CE	1:A:589:PRO:HG3	2.38	0.52
1:B:363:TRP:O	1:B:367:VAL:HG12	2.09	0.52
1:B:731:LYS:N	1:B:732:PRO:CD	2.72	0.52
1:A:90:ASP:CB	1:A:171:LYS:HA	2.39	0.52
1:A:372:LEU:HD23	1:A:372:LEU:N	2.24	0.52
1:A:62:PHE:CD1	1:A:142:TYR:HB2	2.45	0.52
1:B:56:ALA:CB	1:B:61:ARG:CA	2.81	0.52
1:A:384:GLU:HG2	1:A:489:ASN:HB3	1.90	0.52
1:B:932:GLN:HA	1:B:932:GLN:NE2	2.25	0.52
1:B:416:TYR:O	1:B:418:LEU:N	2.43	0.52
1:B:615:PRO:O	1:B:616:GLU:CB	2.57	0.52
1:B:313:TYR:CE2	1:B:478:ILE:HD11	2.43	0.52
1:B:62:PHE:CE1	1:B:142:TYR:HB2	2.44	0.52
1:B:833:HIS:HB2	1:B:836:LYS:HG3	1.92	0.52
1:B:622:LYS:HZ3	1:B:658:ASP:HB3	1.75	0.52
1:A:119:ASN:ND2	8:A:1000:HOH:O	2.43	0.51
1:B:928:LEU:HB2	1:B:930:ILE:HG22	1.92	0.51
1:A:63:PRO:HB3	1:A:107:PHE:CE2	2.45	0.51
1:A:397:LYS:HB3	1:A:459:ALA:HB2	1.91	0.51
1:A:592:TYR:HA	1:A:622:LYS:O	2.10	0.51
1:B:258:LYS:HG2	5:B:1081:NAG:C6	2.38	0.51
1:B:159:HIS:O	1:B:160:LEU:HD22	2.10	0.51
1:A:718:ILE:HD12	1:A:949:LEU:HD11	1.92	0.51
1:B:432:SER:HB3	1:B:936:GLU:OE2	2.10	0.51
1:A:436:ILE:HD11	1:A:457:LYS:HG2	1.92	0.51
1:B:611:THR:HG22	1:B:612:LEU:N	2.25	0.51
1:B:298:TYR:CZ	1:B:361:LYS:HD2	2.46	0.51
1:A:227:GLU:HG3	4:A:1071:NAG:C8	2.40	0.51
1:B:227:GLU:OE1	1:B:229:ARG:HD3	2.11	0.51
1:B:902:THR:OG1	1:B:934:VAL:HG21	2.10	0.51
1:B:468:PHE:CD2	1:B:469:LEU:HG	2.46	0.51
1:B:309:PHE:C	1:B:309:PHE:CD2	2.83	0.51
1:A:405:ASN:O	1:A:409:PRO:HG3	2.11	0.51
1:A:99:VAL:HG12	1:A:100:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:LYS:HZ1	1:B:662:LEU:HG	1.76	0.51
1:A:132:LYS:HB3	1:A:133:PRO:HD2	1.91	0.51
1:B:397:LYS:HB3	1:B:459:ALA:HB2	1.92	0.51
1:B:327:ALA:HB1	1:B:346:GLU:HG2	1.93	0.51
1:A:327:ALA:HB1	1:A:346:GLU:HG2	1.93	0.51
1:B:63:PRO:HB3	1:B:107:PHE:CE2	2.46	0.51
1:B:549:LEU:HB2	1:B:566:PHE:HD2	1.74	0.51
1:A:468:PHE:CD2	1:A:469:LEU:HG	2.45	0.51
1:B:442:THR:HG23	1:B:445:GLN:H	1.75	0.51
1:B:99:VAL:HG12	1:B:100:LEU:H	1.76	0.51
1:B:156:LEU:HD12	1:B:162:TYR:CE1	2.46	0.50
1:A:417:PHE:O	1:A:420:VAL:HB	2.11	0.50
1:B:655:ARG:HB2	1:B:658:ASP:HB2	1.92	0.50
1:B:355:THR:HG21	1:B:817:SER:OG	2.11	0.50
1:B:417:PHE:O	1:B:420:VAL:HB	2.11	0.50
1:A:80:LEU:HD22	1:A:81:PHE:N	2.26	0.50
1:B:932:GLN:HA	1:B:932:GLN:HE21	1.77	0.50
1:B:55:VAL:O	1:B:56:ALA:HB2	2.10	0.50
1:A:466:LYS:HG3	1:A:466:LYS:O	2.11	0.50
1:A:905:PHE:O	1:A:938:ILE:HG23	2.11	0.50
1:A:710:MET:O	1:A:713:ARG:O	2.28	0.50
1:A:697:LEU:HD11	1:A:750:LEU:HD13	1.92	0.50
1:A:432:SER:HB3	1:A:936:GLU:OE2	2.12	0.50
1:A:309:PHE:CD2	1:A:309:PHE:C	2.84	0.50
1:B:372:LEU:N	1:B:372:LEU:HD23	2.26	0.50
1:B:921:LEU:O	1:B:922:GLU:HB2	2.12	0.50
1:A:313:TYR:CE2	1:A:478:ILE:HD11	2.45	0.50
1:B:602:ARG:O	1:B:603:HIS:HB2	2.11	0.50
1:B:258:LYS:CG	5:B:1081:NAG:H62	2.38	0.50
1:B:727:LEU:HD22	1:B:761:LEU:HD23	1.93	0.50
1:B:59:GLY:C	1:B:60:GLU:HG2	2.32	0.50
1:B:730:PHE:C	1:B:732:PRO:HD2	2.32	0.50
1:B:475:GLN:O	1:B:479:ILE:HG12	2.12	0.50
1:A:191:THR:H	1:B:191:THR:HB	1.77	0.50
1:B:866:PRO:O	1:B:869:GLN:HG2	2.11	0.50
1:B:446:ILE:O	1:B:449:MET:HB2	2.12	0.50
1:B:721:ASN:HB3	1:B:956:LEU:HD13	1.93	0.50
1:B:121:THR:HA	1:B:137:LEU:HD23	1.94	0.50
1:B:877:ARG:HA	1:B:917:PHE:CE1	2.46	0.50
1:B:905:PHE:O	1:B:938:ILE:HG23	2.11	0.50
1:B:432:SER:HB3	1:B:936:GLU:CD	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:GLY:O	1:B:926:SER:C	2.50	0.49
1:A:342:ILE:HD11	1:A:375:GLN:NE2	2.27	0.49
1:A:721:ASN:HB3	1:A:956:LEU:HD13	1.93	0.49
1:A:536:GLU:O	1:A:540:THR:HG22	2.12	0.49
1:B:541:TRP:CH2	1:B:548:PRO:HG2	2.47	0.49
1:A:638:HIS:HB2	1:A:642:GLN:HE21	1.76	0.49
1:B:386:TRP:HB3	1:B:446:ILE:HG23	1.95	0.49
1:A:559:LEU:HD12	1:A:612:LEU:O	2.12	0.49
1:A:416:TYR:HE2	1:A:419:ASN:HB2	1.75	0.49
1:B:700:LEU:HD21	1:B:730:PHE:HD1	1.77	0.49
1:B:452:GLU:N	6:B:1084:MES:H61	2.27	0.49
1:B:769:LYS:HD2	1:B:773:LEU:CD1	2.42	0.49
1:B:466:LYS:HG3	1:B:466:LYS:O	2.12	0.49
1:B:838:LEU:O	1:B:842:GLU:HG2	2.12	0.49
1:A:475:GLN:O	1:A:479:ILE:HG12	2.13	0.49
1:A:620:TRP:CE3	1:A:620:TRP:O	2.66	0.49
1:A:602:ARG:O	1:A:603:HIS:HB2	2.11	0.49
1:A:384:GLU:HA	1:A:489:ASN:ND2	2.22	0.49
1:B:236:MET:HB3	1:B:254:GLU:HB3	1.95	0.49
1:B:69:LEU:HD23	1:B:147:GLN:HE21	1.78	0.49
1:A:410:GLU:OE2	1:A:410:GLU:N	2.43	0.49
1:A:56:ALA:CB	1:A:57:THR:CA	2.87	0.49
1:B:918:PHE:CE2	1:B:934:VAL:CG1	2.95	0.49
1:B:718:ILE:CG2	1:B:952:LEU:HD22	2.42	0.49
1:A:718:ILE:CG2	1:A:952:LEU:HD22	2.42	0.49
1:A:432:SER:HB3	1:A:936:GLU:CD	2.33	0.49
1:B:388:ASP:OD2	1:B:492:ASN:HB2	2.13	0.49
1:B:465:LEU:HD23	1:B:474:PHE:HE1	1.78	0.49
1:A:67:LEU:HA	1:A:145:HIS:CD2	2.48	0.49
1:A:93:ALA:HB3	1:A:168:PHE:CE2	2.47	0.49
1:B:640:TRP:CZ3	1:B:666:VAL:HG22	2.48	0.49
1:B:614:LEU:HG	1:B:616:GLU:O	2.12	0.49
1:B:872:ALA:HB1	1:B:901:THR:HG22	1.95	0.49
1:B:934:VAL:CG1	1:B:935:LEU:N	2.75	0.49
1:B:378:GLY:HA2	1:B:392:ASN:OD1	2.12	0.49
1:A:465:LEU:HD23	1:A:474:PHE:HE1	1.78	0.48
1:B:60:GLU:HB2	1:B:61:ARG:CA	2.44	0.48
1:B:681:LEU:HB3	1:B:955:TRP:NE1	2.28	0.48
1:A:693:SER:O	1:A:697:LEU:HB2	2.13	0.48
1:A:911:LEU:HD23	1:A:911:LEU:C	2.34	0.48
1:A:468:PHE:CE2	1:A:469:LEU:HG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:LEU:HD13	1:B:686:TYR:CE2	2.47	0.48
1:A:866:PRO:O	1:A:869:GLN:HG2	2.13	0.48
1:A:626:ASP:HA	1:A:657:LYS:CB	2.36	0.48
1:A:442:THR:HG23	1:A:445:GLN:H	1.79	0.48
1:B:541:TRP:HH2	1:B:548:PRO:HG2	1.78	0.48
1:A:62:PHE:CE1	1:A:142:TYR:HB2	2.49	0.48
1:A:733:VAL:HG13	1:A:734:ILE:N	2.28	0.48
1:B:620:TRP:CE3	1:B:620:TRP:O	2.67	0.48
1:A:366[B]:ARG:NH1	1:A:400:GLU:OE2	2.46	0.48
1:A:541:TRP:CH2	1:A:548:PRO:HG2	2.48	0.48
1:A:363:TRP:O	1:A:367:VAL:HG12	2.13	0.48
1:A:382:THR:O	1:A:489:ASN:HA	2.12	0.48
1:B:547:ILE:HD11	1:B:631:TYR:HA	1.96	0.48
1:B:67:LEU:CA	1:B:145:HIS:HD2	2.27	0.48
1:A:197:THR:HG23	1:A:266:TYR:O	2.14	0.48
1:A:833:HIS:HB2	1:A:836:LYS:HG3	1.94	0.48
1:B:826:TYR:O	1:B:829:SER:HB2	2.14	0.48
1:A:769:LYS:HD2	1:A:773:LEU:CD1	2.44	0.48
1:B:488:ARG:CG	1:B:489:ASN:H	2.26	0.48
1:B:468:PHE:CE2	1:B:469:LEU:HG	2.48	0.48
1:A:701:SER:OG	1:A:702:TYR:N	2.46	0.48
1:B:664:HIS:CD2	1:B:668:GLN:HG3	2.49	0.48
1:A:604:ILE:CD1	1:A:604:ILE:H	2.24	0.48
1:A:838:LEU:CD2	1:A:871:LEU:HD21	2.41	0.48
1:B:314:PHE:C	1:B:479:ILE:HD12	2.34	0.48
1:A:547:ILE:HG12	1:A:548:PRO:CD	2.43	0.48
1:A:738:SER:O	1:A:751:ARG:CD	2.61	0.48
1:B:748:ARG:HB3	1:B:789:ASP:OD2	2.12	0.48
1:B:855:LEU:HD22	1:B:859:LEU:HD22	1.95	0.48
1:B:924:GLN:O	1:B:925:GLY:C	2.51	0.48
1:A:697:LEU:HD12	1:A:697:LEU:HA	1.64	0.48
1:B:72:VAL:CG1	1:B:103:ASN:HB2	2.43	0.48
1:B:880:TRP:HZ2	1:B:889:LEU:HD23	1.79	0.48
1:B:915:LYS:HA	1:B:935:LEU:HD21	1.95	0.47
1:B:918:PHE:CZ	1:B:934:VAL:HG11	2.49	0.47
1:A:72:VAL:CG1	1:A:103:ASN:HB2	2.44	0.47
1:B:828:LEU:HB3	1:B:840:LEU:HD11	1.95	0.47
1:A:659:ARG:NH2	8:A:990:HOH:O	2.45	0.47
1:B:79:ASP:HB2	1:B:96:LYS:HB3	1.96	0.47
1:B:200:GLU:HA	1:B:201:PRO:HA	1.63	0.47
1:A:386:TRP:HB3	1:A:446:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:TRP:CD1	1:B:675:LEU:HD21	2.49	0.47
1:A:86:LEU:HD21	1:A:268:VAL:CG2	2.44	0.47
1:B:80:LEU:HD12	1:B:222:ILE:CD1	2.44	0.47
1:B:945:LEU:HD23	1:B:945:LEU:HA	1.71	0.47
1:A:664:HIS:CD2	1:A:668:GLN:HG3	2.50	0.47
1:A:666:VAL:HG11	1:A:680:ALA:HA	1.97	0.47
1:A:121:THR:HA	1:A:137:LEU:HD23	1.95	0.47
1:A:446:ILE:O	1:A:449:MET:HB2	2.13	0.47
1:A:541:TRP:HH2	1:A:548:PRO:HG2	1.78	0.47
1:B:67:LEU:CA	1:B:145:HIS:CD2	2.98	0.47
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.96	0.47
1:A:156:LEU:HD12	1:A:162:TYR:CE1	2.49	0.47
1:A:730:PHE:C	1:A:732:PRO:HD2	2.35	0.47
1:B:457:LYS:HE3	1:B:630:TYR:HE2	1.79	0.47
1:B:183:THR:HG22	1:B:193:ILE:HG12	1.97	0.47
1:B:140:LEU:CD1	1:B:151:LEU:HD11	2.45	0.47
1:B:697:LEU:HD12	1:B:697:LEU:HA	1.64	0.47
1:B:911:LEU:HD23	1:B:911:LEU:C	2.34	0.47
1:A:236:MET:HB3	1:A:254:GLU:HB3	1.97	0.47
1:B:880:TRP:CZ2	1:B:889:LEU:HD23	2.50	0.47
1:A:457:LYS:HE3	1:A:630:TYR:CE2	2.50	0.47
1:B:659:ARG:HD2	1:B:690:GLU:OE1	2.15	0.47
1:B:275:SER:HB3	1:B:283:LYS:HE2	1.97	0.47
1:A:748:ARG:HB3	1:A:789:ASP:OD2	2.15	0.47
1:B:738:SER:O	1:B:751:ARG:CD	2.63	0.47
1:A:388:ASP:OD2	1:A:492:ASN:HB2	2.15	0.47
1:B:565:ARG:HD3	1:B:567:LEU:HD11	1.96	0.47
1:A:488:ARG:HG2	1:A:489:ASN:N	2.29	0.47
1:A:911:LEU:HD11	1:A:939:THR:HG22	1.96	0.47
1:A:614:LEU:HG	1:A:616:GLU:O	2.15	0.47
1:A:547:ILE:HD11	1:A:631:TYR:HA	1.96	0.47
1:B:183:THR:HG22	1:B:193:ILE:CG1	2.44	0.47
1:A:651:HIS:CD2	1:A:652:THR:N	2.82	0.47
1:A:74:ILE:HA	1:A:75:PRO:HD3	1.72	0.47
3:B:968:LYS:HB3	6:B:1084:MES:O1S	2.15	0.47
1:A:183:THR:HG22	1:A:193:ILE:CG1	2.44	0.47
1:A:79:ASP:HB2	1:A:96:LYS:HB3	1.97	0.47
1:A:90:ASP:HB2	1:A:170:ALA:O	2.15	0.47
1:A:533:GLU:HG3	1:A:536:GLU:OE2	2.14	0.46
1:A:801:THR:HG23	1:A:804:GLY:N	2.23	0.46
1:A:770:ALA:CB	1:A:797:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ALA:CB	1:B:797:VAL:HG21	2.45	0.46
1:B:774:PHE:HB2	1:B:794:VAL:HG12	1.97	0.46
1:B:223:LYS:HD3	1:B:252:HIS:CE1	2.50	0.46
1:A:544:GLN:NE2	1:A:584:TYR:CD1	2.76	0.46
1:A:662:LEU:HB3	1:A:683:MET:HE1	1.97	0.46
1:B:278:THR:HG23	1:B:282:VAL:N	2.29	0.46
1:B:86:LEU:HD21	1:B:268:VAL:CG2	2.44	0.46
1:B:894:ILE:HD13	1:B:894:ILE:HA	1.75	0.46
1:A:932:GLN:NE2	1:A:932:GLN:HA	2.30	0.46
1:B:536:GLU:O	1:B:540:THR:HG22	2.14	0.46
1:B:104:ALA:CB	1:B:158:PRO:HD3	2.44	0.46
1:A:55:VAL:CB	1:A:62:PHE:HB2	2.46	0.46
1:A:659:ARG:HD2	1:A:690:GLU:OE1	2.16	0.46
1:B:235:ASN:ND2	1:B:263:LEU:O	2.47	0.46
1:A:124:SER:CB	1:A:131:MET:H	2.28	0.46
1:A:640:TRP:CZ3	1:A:666:VAL:HG22	2.51	0.46
1:A:902:THR:OG1	1:A:934:VAL:HG21	2.16	0.46
1:B:442:THR:HG21	8:B:984:HOH:O	2.14	0.46
1:A:314:PHE:O	1:A:316:ILE:HG13	2.16	0.46
1:B:93:ALA:HB3	1:B:168:PHE:CE2	2.51	0.46
1:B:544:GLN:NE2	1:B:584:TYR:CD1	2.76	0.46
1:A:680:ALA:O	1:A:684:THR:HG23	2.15	0.46
1:A:681:LEU:HB3	1:A:955:TRP:NE1	2.31	0.46
1:B:724:ARG:O	1:B:728:GLN:HB2	2.15	0.46
1:A:826:TYR:O	1:A:829:SER:HB2	2.15	0.46
1:A:106:GLN:HE21	1:A:155:LYS:NZ	2.13	0.46
1:A:537:MET:O	1:A:540:THR:CG2	2.61	0.46
1:B:537:MET:O	1:B:540:THR:CG2	2.62	0.46
1:B:148:ILE:HG13	1:B:148:ILE:O	2.15	0.46
1:B:553:LYS:O	1:B:559:LEU:HA	2.16	0.46
1:B:680:ALA:O	1:B:684:THR:HG23	2.14	0.46
1:B:838:LEU:CD2	1:B:871:LEU:HD21	2.44	0.46
1:A:528:LEU:CB	1:A:529:GLY:HA2	2.37	0.46
1:B:67:LEU:HA	1:B:145:HIS:CD2	2.46	0.46
6:B:1084:MES:H32	6:B:1084:MES:H81	1.44	0.46
1:A:192:ARG:HA	1:B:190:GLU:HG2	1.97	0.46
1:B:559:LEU:HD12	1:B:612:LEU:O	2.15	0.46
1:B:911:LEU:HD11	1:B:939:THR:HG22	1.97	0.46
1:A:889:LEU:HD13	1:A:928:LEU:HD21	1.98	0.46
1:B:488:ARG:HG2	1:B:489:ASN:N	2.29	0.46
1:B:784:LEU:CD1	1:B:786:ILE:HD12	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:LYS:HA	1:A:935:LEU:HD21	1.98	0.46
1:B:640:TRP:O	1:B:644:ILE:HG13	2.15	0.46
1:B:401:LEU:HD23	1:B:402:ILE:N	2.30	0.46
1:B:870:GLN:O	1:B:871:LEU:C	2.54	0.46
1:B:918:PHE:HE2	1:B:934:VAL:CG1	2.29	0.46
1:B:314:PHE:O	1:B:479:ILE:HG23	2.16	0.46
1:A:880:TRP:HZ2	1:A:889:LEU:HD23	1.81	0.46
1:B:604:ILE:C	8:B:1014:HOH:O	2.54	0.46
1:B:693:SER:O	1:B:697:LEU:HB2	2.16	0.46
1:A:725:TYR:CE1	1:A:729:TYR:HD1	2.34	0.46
1:B:945:LEU:O	1:B:949:LEU:N	2.47	0.46
1:B:60:GLU:HB2	1:B:61:ARG:HA	1.98	0.45
1:B:417:PHE:CE1	1:B:421:CYS:SG	3.09	0.45
1:A:793:ILE:O	1:A:797:VAL:HG23	2.16	0.45
1:A:80:LEU:HD22	1:A:81:PHE:H	1.81	0.45
1:B:95:GLU:HG2	1:B:168:PHE:HE1	1.81	0.45
1:A:238:LYS:HB3	1:A:238:LYS:HE2	1.81	0.45
1:B:140:LEU:O	1:B:148:ILE:HA	2.16	0.45
1:B:919:GLU:O	1:B:922:GLU:HB2	2.17	0.45
1:A:863:ALA:HB1	1:A:904:HIS:CE1	2.51	0.45
1:B:316:ILE:HD11	1:B:483:LYS:HG3	1.98	0.45
1:B:729:TYR:O	1:B:730:PHE:HB2	2.15	0.45
1:A:784:LEU:CD1	1:A:786:ILE:HD12	2.47	0.45
1:A:928:LEU:HB2	1:A:930:ILE:HG22	1.98	0.45
1:B:651:HIS:CD2	1:B:652:THR:N	2.84	0.45
1:A:411:LEU:HA	1:A:745:VAL:HG21	1.98	0.45
1:A:870:GLN:O	1:A:871:LEU:C	2.54	0.45
1:A:892:TYR:CE1	6:A:1083:MES:H31	2.51	0.45
1:A:647:LEU:HD13	1:A:686:TYR:CE2	2.51	0.45
1:B:570:VAL:HG22	1:B:943:LYS:NZ	2.31	0.45
1:B:911:LEU:O	1:B:915:LYS:HB2	2.17	0.45
1:A:911:LEU:O	1:A:915:LYS:HB2	2.16	0.45
1:B:145:HIS:O	1:B:147:GLN:HG3	2.15	0.45
1:B:638:HIS:HB2	1:B:642:GLN:HE21	1.80	0.45
1:B:202:THR:OG1	1:B:202:THR:O	2.29	0.45
1:B:382:THR:O	1:B:489:ASN:HA	2.16	0.45
1:B:675:LEU:HA	1:B:675:LEU:HD12	1.74	0.45
1:B:725:TYR:CE1	1:B:729:TYR:HD1	2.35	0.45
1:B:793:ILE:O	1:B:797:VAL:HG23	2.16	0.45
1:A:141:SER:O	1:A:143:PRO:HD3	2.16	0.45
1:A:140:LEU:O	1:A:148:ILE:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:MET:HE2	1:A:589:PRO:HG3	1.98	0.45
1:B:537:MET:HG3	1:B:587:HIS:O	2.16	0.45
1:A:553:LYS:O	1:A:559:LEU:HA	2.17	0.45
1:A:200:GLU:HA	1:A:201:PRO:HA	1.65	0.45
1:A:100:LEU:HD12	1:A:101:VAL:O	2.15	0.45
1:B:238:LYS:HE2	1:B:238:LYS:HB3	1.75	0.45
1:B:860:HIS:O	1:B:860:HIS:CD2	2.68	0.45
1:B:557:CYS:SG	1:B:617:LYS:CG	3.05	0.45
1:A:337:GLU:HA	1:A:342:ILE:HG12	1.98	0.45
1:B:659:ARG:O	1:B:663:ILE:HG13	2.17	0.45
1:B:122:LEU:N	1:B:137:LEU:HD23	2.31	0.45
1:B:592:TYR:OH	1:B:612:LEU:HD21	2.17	0.45
1:B:667:PHE:CE2	1:B:680:ALA:HB1	2.52	0.45
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.60	0.45
1:B:100:LEU:HD12	1:B:101:VAL:O	2.17	0.45
1:B:451:ASP:C	6:B:1084:MES:H61	2.38	0.44
1:A:123:GLN:HE22	1:A:133:PRO:HB3	1.81	0.44
1:A:183:THR:HG22	1:A:193:ILE:HG12	1.98	0.44
1:B:651:HIS:HE1	1:B:689:HIS:O	2.00	0.44
1:B:155:LYS:HB2	1:B:155:LYS:HE2	1.76	0.44
1:B:89:LEU:HD13	1:B:181:LYS:HD3	1.99	0.44
1:A:838:LEU:O	1:A:842:GLU:HG2	2.17	0.44
1:A:159:HIS:O	1:A:160:LEU:HD22	2.18	0.44
1:A:537:MET:HE2	1:A:589:PRO:CD	2.47	0.44
1:B:764:ALA:HB3	1:B:765:PRO:HD3	1.99	0.44
1:A:713:ARG:CG	1:A:713:ARG:HH11	2.30	0.44
1:A:918:PHE:CE2	1:A:934:VAL:CG1	2.99	0.44
1:A:949:LEU:HB3	1:A:950:PRO:CD	2.47	0.44
1:B:122:LEU:N	1:B:137:LEU:CD2	2.81	0.44
1:A:442:THR:O	1:A:446:ILE:HG13	2.17	0.44
1:A:442:THR:HG23	1:A:445:GLN:CG	2.45	0.44
1:B:860:HIS:CD2	1:B:860:HIS:C	2.91	0.44
1:A:257:VAL:HG23	1:A:258:LYS:O	2.18	0.44
1:B:160:LEU:HA	1:B:160:LEU:HD13	1.62	0.44
1:A:67:LEU:CA	1:A:145:HIS:CD2	3.01	0.44
1:A:80:LEU:HD12	1:A:222:ILE:HD13	1.98	0.44
1:B:884:LEU:HD12	1:B:884:LEU:HA	1.70	0.44
1:B:889:LEU:O	1:B:889:LEU:HD12	2.17	0.44
1:B:738:SER:O	1:B:751:ARG:HD3	2.18	0.44
1:A:357:SER:O	1:A:360:ASP:HB2	2.17	0.44
1:B:385:TRP:CB	8:B:1013:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:HIS:NE2	1:B:668:GLN:HG3	2.33	0.44
1:A:463:ASN:HB3	8:A:1012:HOH:O	2.18	0.44
1:B:682:ASP:O	1:B:685:TYR:HD2	2.01	0.44
1:A:640:TRP:CD1	1:A:675:LEU:HD21	2.52	0.44
1:B:727:LEU:O	1:B:731:LYS:HB2	2.18	0.44
1:A:320:LEU:HD23	1:A:320:LEU:N	2.33	0.44
1:B:331:PHE:CD1	1:B:333:PRO:HD2	2.53	0.44
1:A:227:GLU:HG3	4:A:1071:NAG:H82	2.00	0.44
1:B:106:GLN:HE21	1:B:155:LYS:NZ	2.16	0.44
1:A:769:LYS:HD2	1:A:773:LEU:HD13	2.00	0.43
1:B:385:TRP:CG	1:B:386:TRP:N	2.86	0.43
1:A:640:TRP:O	1:A:644:ILE:HG13	2.17	0.43
1:B:666:VAL:HG11	1:B:680:ALA:HA	1.99	0.43
1:B:838:LEU:HD13	1:B:842:GLU:CG	2.48	0.43
1:A:314:PHE:C	1:A:479:ILE:HD12	2.37	0.43
4:A:1071:NAG:H62	4:A:1072:NAG:C1	2.48	0.43
1:B:714:ASN:O	1:B:716:SER:N	2.51	0.43
1:A:293:ARG:NH2	7:B:1079:MAN:O2	2.51	0.43
1:A:140:LEU:CD1	1:A:151:LEU:HD11	2.49	0.43
1:B:566:PHE:C	1:B:567:LEU:HD12	2.38	0.43
1:B:352:ASP:HA	1:B:353:PRO:HD3	1.82	0.43
1:B:730:PHE:O	1:B:733:VAL:HG12	2.18	0.43
1:A:918:PHE:CZ	1:A:934:VAL:HG11	2.53	0.43
1:A:314:PHE:HA	1:A:479:ILE:CD1	2.49	0.43
1:A:932:GLN:HE21	1:A:932:GLN:HA	1.84	0.43
1:A:880:TRP:CZ2	1:A:889:LEU:HD23	2.52	0.43
1:A:223:LYS:HD3	1:A:252:HIS:CE1	2.53	0.43
1:A:245:GLU:CG	1:A:246:GLY:N	2.74	0.43
1:A:122:LEU:N	1:A:137:LEU:HD23	2.33	0.43
1:B:634:HIS:CE1	1:B:674:ARG:HB3	2.54	0.43
1:A:488:ARG:CG	1:A:489:ASN:H	2.27	0.43
1:B:159:HIS:C	1:B:160:LEU:HD22	2.38	0.43
1:A:159:HIS:C	1:A:160:LEU:HD22	2.39	0.43
1:B:860:HIS:NE2	1:B:864:ARG:HD2	2.33	0.43
1:B:434:ARG:HB2	1:B:435:PRO:CD	2.47	0.43
1:B:650:ASN:HB3	1:B:653:LEU:HG	2.00	0.43
1:B:622:LYS:HZ3	1:B:658:ASP:CB	2.31	0.43
1:B:104:ALA:H	1:B:158:PRO:HG3	1.82	0.43
1:A:342:ILE:HG22	1:A:344:TYR:CE1	2.53	0.43
1:A:155:LYS:HB2	1:A:155:LYS:HE2	1.81	0.43
1:B:701:SER:OG	1:B:702:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD11	1:A:149:ALA:HB2	1.99	0.43
1:A:581:GLN:HB3	1:A:582:GLU:H	1.54	0.43
1:A:537:MET:HE2	1:A:589:PRO:HD3	2.01	0.43
1:A:592:TYR:OH	1:A:612:LEU:HD21	2.19	0.43
1:A:622:LYS:HZ3	1:A:658:ASP:HB3	1.83	0.43
1:B:733:VAL:HG13	1:B:734:ILE:N	2.33	0.43
1:B:717:ASP:OD2	1:B:718:ILE:HG13	2.19	0.43
1:A:889:LEU:HA	1:A:890:GLY:HA2	1.54	0.43
1:B:385:TRP:CG	8:B:1013:HOH:O	2.68	0.43
1:B:75:PRO:CG	1:B:211:PHE:CD1	2.96	0.43
1:B:551:VAL:HG22	1:B:562:GLN:O	2.18	0.43
1:B:625:VAL:O	1:B:626:ASP:HB2	2.19	0.43
1:B:910:LYS:HA	1:B:913:GLU:HG3	2.00	0.43
1:B:320:LEU:N	1:B:320:LEU:HD23	2.33	0.43
1:A:860:HIS:O	1:A:860:HIS:CD2	2.72	0.43
1:A:889:LEU:HD12	1:A:889:LEU:O	2.18	0.43
1:A:126:GLU:O	1:A:160:LEU:HD12	2.19	0.43
1:B:90:ASP:HB2	1:B:170:ALA:O	2.19	0.43
1:B:323:LEU:HD13	1:B:340:GLY:HA2	2.00	0.43
1:A:142:TYR:CZ	1:A:144:ALA:HB3	2.54	0.43
1:A:202:THR:OG1	1:A:202:THR:O	2.32	0.43
1:B:622:LYS:HZ2	1:B:662:LEU:HG	1.83	0.43
1:A:314:PHE:O	1:A:479:ILE:HD12	2.19	0.43
1:B:907:SER:O	1:B:942:ILE:HD11	2.19	0.43
1:B:184:TYR:HB2	8:B:973:HOH:O	2.18	0.43
1:B:74:ILE:HA	1:B:75:PRO:HD3	1.73	0.43
1:A:401:LEU:HD23	1:A:402:ILE:N	2.34	0.43
1:A:620:TRP:C	1:A:620:TRP:CE3	2.92	0.43
1:B:943:LYS:O	1:B:944:TRP:C	2.58	0.43
1:B:357:SER:O	1:B:360:ASP:HB2	2.18	0.43
1:A:378:GLY:HA2	1:A:392:ASN:OD1	2.19	0.43
1:A:587:HIS:CE1	1:A:606:LYS:HD3	2.54	0.42
1:B:567:LEU:HD12	1:B:567:LEU:N	2.33	0.42
1:B:634:HIS:NE2	1:B:674:ARG:HB3	2.33	0.42
1:A:145:HIS:O	1:A:147:GLN:HG3	2.19	0.42
1:A:738:SER:O	1:A:751:ARG:HD3	2.18	0.42
1:A:954:THR:O	1:A:958:VAL:HG23	2.19	0.42
1:B:355:THR:O	1:B:355:THR:CG2	2.66	0.42
1:A:741:ASP:OD2	1:A:787:PRO:CB	2.61	0.42
1:A:313:TYR:O	1:A:479:ILE:HD11	2.19	0.42
1:B:566:PHE:CZ	1:B:672:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:HD13	1:A:842:GLU:CG	2.49	0.42
1:A:764:ALA:HB3	1:A:765:PRO:HD3	2.01	0.42
1:B:240:LYS:HB3	1:B:240:LYS:HE2	1.75	0.42
1:B:938:ILE:O	1:B:941:ASN:HB2	2.19	0.42
1:B:949:LEU:HB3	1:B:950:PRO:CD	2.48	0.42
1:B:884:LEU:HD11	1:B:889:LEU:HB3	2.01	0.42
1:B:647:LEU:HD21	1:B:659:ARG:HG2	2.01	0.42
1:B:465:LEU:HD22	1:B:496:TRP:CZ3	2.52	0.42
1:A:419:ASN:N	1:A:419:ASN:HD22	2.17	0.42
1:A:547:ILE:HA	1:A:548:PRO:HD3	1.90	0.42
1:B:441:GLU:N	1:B:445:GLN:OE1	2.50	0.42
1:B:718:ILE:HG21	1:B:952:LEU:HD22	2.02	0.42
1:A:659:ARG:O	1:A:663:ILE:HG13	2.20	0.42
1:B:670:VAL:HG12	1:B:948:ASN:ND2	2.35	0.42
1:A:385:TRP:CG	1:A:386:TRP:N	2.86	0.42
1:B:419:ASN:O	1:B:423:GLU:HG3	2.20	0.42
1:B:412:GLN:HB2	1:B:746:TRP:HE1	1.85	0.42
1:B:422:PHE:O	1:B:425:ILE:HB	2.19	0.42
1:A:921:LEU:O	1:A:922:GLU:HB2	2.19	0.42
1:A:57:THR:HG23	1:A:141:SER:O	2.20	0.42
1:B:386:TRP:CE3	1:B:389:ILE:HD13	2.55	0.42
1:A:551:VAL:HG22	1:A:562:GLN:O	2.20	0.42
1:B:466:LYS:HB2	1:B:474:PHE:CD2	2.54	0.42
1:B:765:PRO:O	1:B:768:GLN:HB2	2.20	0.42
1:B:313:TYR:O	1:B:479:ILE:HD11	2.20	0.42
1:A:288:ALA:O	1:A:289:SER:C	2.58	0.42
1:A:113:LYS:HG3	1:A:114:ASP:OD1	2.19	0.42
1:B:213:GLU:HB2	1:B:216:PHE:HD2	1.85	0.42
1:B:412:GLN:HB2	1:B:746:TRP:NE1	2.34	0.42
1:A:750:LEU:HD12	1:A:754:LEU:HG	2.02	0.42
1:A:566:PHE:CD2	1:A:632:ILE:HD12	2.55	0.42
1:A:774:PHE:HB2	1:A:794:VAL:HG12	2.01	0.42
1:A:729:TYR:O	1:A:730:PHE:HB2	2.20	0.42
1:A:884:LEU:HD11	1:A:889:LEU:HB3	2.01	0.42
1:B:497:SER:OG	1:B:535:LYS:HE3	2.18	0.42
1:A:153:PRO:O	1:A:154:GLU:HG3	2.20	0.42
1:B:239:VAL:CG1	1:B:240:LYS:HE3	2.48	0.42
1:A:934:VAL:HG12	1:A:935:LEU:N	2.35	0.42
1:A:669:LEU:HA	1:A:669:LEU:HD23	1.92	0.42
1:A:271:PHE:CD2	1:A:288:ALA:HA	2.55	0.42
1:A:945:LEU:HD23	1:A:945:LEU:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:LEU:HA	1:A:675:LEU:HD12	1.73	0.41
1:A:122:LEU:CB	1:A:137:LEU:HD21	2.50	0.41
1:B:402:ILE:HG12	1:B:402:ILE:H	1.57	0.41
1:B:693:SER:N	1:B:694:PRO:CD	2.82	0.41
1:A:919:GLU:O	1:A:922:GLU:CB	2.68	0.41
1:B:647:LEU:HD23	1:B:647:LEU:HA	1.78	0.41
1:A:82:VAL:O	1:A:84:PRO:HD3	2.20	0.41
1:B:141:SER:O	1:B:143:PRO:HD3	2.19	0.41
1:B:784:LEU:HD12	1:B:786:ILE:HD12	2.01	0.41
1:A:935:LEU:O	1:A:939:THR:HG23	2.19	0.41
1:B:588:ILE:O	1:B:588:ILE:HG23	2.21	0.41
1:B:105:THR:O	1:B:156:LEU:HD23	2.19	0.41
1:A:401:LEU:HD12	1:A:417:PHE:CG	2.55	0.41
1:B:67:LEU:HD12	1:B:68:ARG:N	2.34	0.41
1:B:739:TRP:CE2	1:B:769:LYS:HG2	2.55	0.41
1:A:201:PRO:HD2	1:A:202:THR:H	1.84	0.41
1:A:485:PHE:O	1:A:486:SER:C	2.57	0.41
1:A:537:MET:HG3	1:A:587:HIS:O	2.20	0.41
1:B:600:ILE:CD1	1:B:625:VAL:HG21	2.50	0.41
1:B:662:LEU:HB3	1:B:683:MET:CE	2.50	0.41
1:A:723:LYS:HG3	1:A:761:LEU:HG	2.02	0.41
1:B:750:LEU:HD12	1:B:754:LEU:HG	2.01	0.41
1:A:277:PHE:HA	1:A:282:VAL:O	2.21	0.41
1:B:721:ASN:ND2	1:B:724:ARG:HH12	2.19	0.41
1:B:769:LYS:HD2	1:B:773:LEU:HD13	2.00	0.41
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.87	0.41
1:A:565:ARG:NH1	1:A:581:GLN:HB2	2.33	0.41
1:B:549:LEU:HB2	1:B:566:PHE:CD2	2.55	0.41
1:A:122:LEU:N	1:A:137:LEU:CD2	2.83	0.41
1:B:605:LEU:HD11	1:B:607:SER:O	2.20	0.41
1:A:809:LEU:O	1:A:812:TYR:HB3	2.20	0.41
1:B:366:ARG:NH1	1:B:416:TYR:CE1	2.89	0.41
1:B:318:TYR:CZ	1:B:320:LEU:HB2	2.55	0.41
1:A:860:HIS:NE2	1:A:864:ARG:HD2	2.35	0.41
1:B:620:TRP:CE3	1:B:620:TRP:C	2.93	0.41
1:A:302:ALA:O	1:A:303:SER:C	2.59	0.41
1:B:122:LEU:CB	1:B:137:LEU:HD21	2.49	0.41
1:B:917:PHE:O	1:B:920:SER:HB3	2.20	0.41
1:A:104:ALA:CB	1:A:158:PRO:HD3	2.47	0.41
1:B:282:VAL:HG21	1:B:318:TYR:HD2	1.86	0.41
1:A:83:HIS:CD2	1:A:225:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:HB2	1:B:61:ARG:HB3	2.02	0.41
1:A:662:LEU:HA	1:A:662:LEU:HD23	1.92	0.41
1:A:69:LEU:HD23	1:A:147:GLN:HE21	1.85	0.41
1:A:314:PHE:CE1	1:A:377:PHE:HE2	2.38	0.41
1:B:183:THR:HA	1:B:192:ARG:O	2.21	0.41
1:A:717:ASP:OD2	1:A:718:ILE:HG13	2.20	0.41
1:B:537:MET:HA	1:B:587:HIS:HB2	2.02	0.41
1:A:75:PRO:CG	1:A:211:PHE:CD1	2.95	0.41
1:B:935:LEU:O	1:B:939:THR:HG23	2.21	0.41
1:B:314:PHE:CE1	1:B:377:PHE:HE2	2.39	0.41
1:B:889:LEU:HD12	1:B:889:LEU:C	2.41	0.41
1:B:327:ALA:HB2	1:B:349:LEU:HD23	2.03	0.41
1:A:943:LYS:O	1:A:944:TRP:C	2.58	0.41
1:A:882:HIS:NE2	1:A:886:LYS:HE2	2.36	0.41
1:B:153:PRO:O	1:B:154:GLU:HG3	2.20	0.41
1:B:801:THR:HG23	1:B:804:GLY:N	2.24	0.41
1:B:424:VAL:HG13	1:B:425:ILE:N	2.36	0.41
1:A:693:SER:N	1:A:694:PRO:CD	2.84	0.41
1:A:67:LEU:CA	1:A:145:HIS:HD2	2.29	0.41
1:A:67:LEU:HD12	1:A:68:ARG:N	2.36	0.41
1:B:408:TYR:N	1:B:409:PRO:HD3	2.36	0.41
1:A:860:HIS:C	1:A:860:HIS:CD2	2.94	0.41
1:B:889:LEU:HA	1:B:890:GLY:HA2	1.56	0.41
1:B:889:LEU:HD13	1:B:928:LEU:HD21	2.03	0.41
1:A:664:HIS:NE2	1:A:668:GLN:HG3	2.35	0.41
1:A:497:SER:OG	1:A:535:LYS:HE3	2.21	0.41
1:A:660:VAL:HG12	1:A:661:GLY:N	2.35	0.41
1:B:726:LEU:HA	1:B:726:LEU:HD23	1.84	0.41
1:B:741:ASP:OD2	1:B:787:PRO:CB	2.63	0.41
1:B:924:GLN:HG3	1:B:925:GLY:N	2.36	0.41
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.55	0.41
1:B:779:GLU:HG2	1:B:779:GLU:O	2.21	0.41
1:B:636:GLU:HG3	1:B:636:GLU:H	1.69	0.41
1:B:113:LYS:HG3	1:B:114:ASP:OD1	2.21	0.41
1:B:559:LEU:HD12	1:B:612:LEU:HB3	2.02	0.40
1:B:604:ILE:CD1	1:B:604:ILE:H	2.23	0.40
1:A:318:TYR:HA	1:A:319:PRO:HD3	1.76	0.40
1:B:325:LEU:HD23	1:B:344:TYR:CE1	2.56	0.40
1:A:949:LEU:N	1:A:950:PRO:HD2	2.36	0.40
1:B:739:TRP:CZ2	1:B:755:LEU:HD22	2.56	0.40
1:A:95:GLU:HG2	1:A:168:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:CZ	1:A:320:LEU:HB2	2.56	0.40
1:A:323:LEU:HD13	1:A:340:GLY:HA2	2.04	0.40
1:A:331:PHE:CD1	1:A:333:PRO:HD2	2.56	0.40
1:A:63:PRO:HB3	1:A:107:PHE:CD2	2.56	0.40
1:B:462:LEU:HD23	1:B:462:LEU:HA	1.90	0.40
1:B:431:ASN:HA	1:B:565:ARG:NH2	2.37	0.40
1:B:662:LEU:HB3	1:B:683:MET:HE1	2.02	0.40
1:B:640:TRP:CZ3	1:B:662:LEU:HD22	2.55	0.40
1:B:677:LEU:HB3	1:B:951:THR:CG2	2.51	0.40
1:A:813:GLU:OE1	1:B:848:LYS:NZ	2.55	0.40
1:A:650:ASN:HB3	1:A:653:LEU:HG	2.04	0.40
1:A:598:ASN:HD22	1:A:598:ASN:C	2.25	0.40
1:B:121:THR:CA	1:B:137:LEU:HD23	2.51	0.40
1:A:105:THR:O	1:A:156:LEU:HD23	2.22	0.40
1:A:441:GLU:N	1:A:445:GLN:OE1	2.52	0.40
1:B:605:LEU:HB3	8:B:1014:HOH:O	2.21	0.40
1:A:419:ASN:O	1:A:423:GLU:HG3	2.22	0.40
1:A:412:GLN:HB2	1:A:746:TRP:NE1	2.37	0.40
1:B:337:GLU:O	1:B:338:ASN:C	2.59	0.40
1:B:99:VAL:HG12	1:B:100:LEU:N	2.35	0.40
1:B:336:MET:HB3	1:B:343:THR:OG1	2.21	0.40
1:B:439:PRO:HB2	8:B:994:HOH:O	2.22	0.40
1:A:894:ILE:HA	1:A:894:ILE:HD13	1.80	0.40
1:A:877:ARG:HB3	1:A:877:ARG:HE	1.59	0.40
1:B:419:ASN:HD22	1:B:419:ASN:N	2.19	0.40
1:B:750:LEU:HD11	1:B:754:LEU:HD11	2.04	0.40
1:B:918:PHE:CD2	1:B:931:PHE:CD1	3.10	0.40
1:A:99:VAL:HG12	1:A:100:LEU:N	2.37	0.40
1:A:889:LEU:C	1:A:889:LEU:HD12	2.41	0.40
1:B:120:ALA:HA	1:B:165:ALA:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	863/967 (89%)	746 (86%)	95 (11%)	22 (2%)	7	33
1	B	851/967 (88%)	732 (86%)	89 (10%)	30 (4%)	4	25
All	All	1714/1934 (89%)	1478 (86%)	184 (11%)	52 (3%)	5	28

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	245	GLU
1	A	417	PHE
1	A	596	SER
1	A	616	GLU
1	A	715	ILE
1	A	922	GLU
1	A	923	ALA
1	B	245	GLU
1	B	417	PHE
1	B	569	GLY
1	B	596	SER
1	B	616	GLU
1	B	715	ILE
1	B	922	GLU
1	B	924	GLN
1	B	926	SER
1	A	216	PHE
1	A	545	LYS
1	A	603	HIS
1	A	925	GLY
1	B	216	PHE
1	B	603	HIS
1	B	925	GLY
1	A	619	SER
1	A	628	ASN
1	A	921	LEU
1	B	60	GLU
1	B	155	LYS
1	B	545	LYS
1	B	628	ASN
1	B	763	HIS
1	A	155	LYS

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Mol	Chain	Res	Type
1	A	535	LYS
1	B	56	ALA
1	B	379	ASN
1	B	535	LYS
1	B	619	SER
1	B	921	LEU
1	B	927	HIS
1	A	764	ALA
1	A	765	PRO
1	A	932	GLN
1	B	764	ALA
1	B	765	PRO
1	A	379	ASN
1	A	763	HIS
1	B	337	GLU
1	B	712	ARG
1	B	943	LYS
1	B	615	PRO
1	B	201	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	773/870 (89%)	677 (88%)	96 (12%)	6	23
1	B	770/870 (88%)	672 (87%)	98 (13%)	5	22
All	All	1543/1740 (89%)	1349 (87%)	194 (13%)	6	22

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	72	VAL
1	A	79	ASP
1	A	87	THR

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Mol	Chain	Res	Type
1	A	94	SER
1	A	100	LEU
1	A	109	ILE
1	A	110	LEU
1	A	124	SER
1	A	125	GLU
1	A	160	LEU
1	A	166	MET
1	A	181	LYS
1	A	193	ILE
1	A	197	THR
1	A	202	THR
1	A	215	LEU
1	A	231	ILE
1	A	278	THR
1	A	285	SER
1	A	289	SER
1	A	320	LEU
1	A	321	SER
1	A	322	LYS
1	A	352	ASP
1	A	355	THR
1	A	364	VAL
1	A	366[A]	ARG
1	A	366[B]	ARG
1	A	367	VAL
1	A	372	LEU
1	A	382	THR
1	A	383	MET
1	A	395	PHE
1	A	416	TYR
1	A	419	ASN
1	A	442	THR
1	A	466	LYS
1	A	469	LEU
1	A	478	ILE
1	A	493	ASP
1	A	533	GLU
1	A	540	THR
1	A	547	ILE
1	A	558	SER
1	A	559	LEU

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Mol	Chain	Res	Type
1	A	560	ARG
1	A	581	GLN
1	A	582	GLU
1	A	583	ARG
1	A	585	LEU
1	A	591	THR
1	A	598	ASN
1	A	604	ILE
1	A	605	LEU
1	A	610	ASP
1	A	618	THR
1	A	621	VAL
1	A	632	ILE
1	A	636	GLU
1	A	641	ASP
1	A	645	THR
1	A	649	GLN
1	A	660	VAL
1	A	675	LEU
1	A	684	THR
1	A	686	TYR
1	A	697	LEU
1	A	701	SER
1	A	705	SER
1	A	713	ARG
1	A	720	GLU
1	A	721	ASN
1	A	729	TYR
1	A	730	PHE
1	A	741	ASP
1	A	750	LEU
1	A	761	LEU
1	A	766	CYS
1	A	767	ILE
1	A	769	LYS
1	A	791	LEU
1	A	825	LEU
1	A	828	LEU
1	A	855	LEU
1	A	859	LEU
1	A	865	ARG
1	A	871	LEU

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Mol	Chain	Res	Type
1	A	889	LEU
1	A	895	ARG
1	A	911	LEU
1	A	916	LEU
1	A	922	GLU
1	A	927	HIS
1	A	933	THR
1	A	934	VAL
1	B	58	ASN
1	B	61	ARG
1	B	72	VAL
1	B	79	ASP
1	B	87	THR
1	B	94	SER
1	B	100	LEU
1	B	109	ILE
1	B	110	LEU
1	B	124	SER
1	B	160	LEU
1	B	166	MET
1	B	181	LYS
1	B	193	ILE
1	B	194	LEU
1	B	197	THR
1	B	202	THR
1	B	215	LEU
1	B	229	ARG
1	B	231	ILE
1	B	278	THR
1	B	285	SER
1	B	289	SER
1	B	320	LEU
1	B	321	SER
1	B	322	LYS
1	B	352	ASP
1	B	355	THR
1	B	364	VAL
1	B	367	VAL
1	B	372	LEU
1	B	382	THR
1	B	383	MET
1	B	395	PHE

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Mol	Chain	Res	Type
1	B	416	TYR
1	B	419	ASN
1	B	442	THR
1	B	466	LYS
1	B	469	LEU
1	B	478	ILE
1	B	493	ASP
1	B	533	GLU
1	B	540	THR
1	B	547	ILE
1	B	558	SER
1	B	559	LEU
1	B	560	ARG
1	B	570	VAL
1	B	583	ARG
1	B	585	LEU
1	B	591	THR
1	B	598	ASN
1	B	604	ILE
1	B	605	LEU
1	B	609	THR
1	B	610	ASP
1	B	618	THR
1	B	621	VAL
1	B	632	ILE
1	B	636	GLU
1	B	645	THR
1	B	649	GLN
1	B	660	VAL
1	B	675	LEU
1	B	684	THR
1	B	686	TYR
1	B	697	LEU
1	B	701	SER
1	B	713	ARG
1	B	720	GLU
1	B	721	ASN
1	B	728	GLN
1	B	729	TYR
1	B	730	PHE
1	B	741	ASP
1	B	750	LEU

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Mol	Chain	Res	Type
1	B	761	LEU
1	B	766	CYS
1	B	767	ILE
1	B	769	LYS
1	B	791	LEU
1	B	825	LEU
1	B	828	LEU
1	B	855	LEU
1	B	859	LEU
1	B	865	ARG
1	B	871	LEU
1	B	889	LEU
1	B	895	ARG
1	B	901	THR
1	B	911	LEU
1	B	916	LEU
1	B	922	GLU
1	B	927	HIS
1	B	932	GLN
1	B	933	THR
1	B	934	VAL
1	B	940	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	106	GLN
1	A	119	ASN
1	A	123	GLN
1	A	145	HIS
1	A	147	GLN
1	A	159	HIS
1	A	169	GLN
1	A	230	HIS
1	A	272	HIS
1	A	297	HIS
1	A	419	ASN
1	A	489	ASN
1	A	544	GLN
1	A	598	ASN
1	A	624	ASN

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Mol	Chain	Res	Type
1	A	642	GLN
1	A	651	HIS
1	A	721	ASN
1	A	811	GLN
1	A	833	HIS
1	A	860	HIS
1	A	869	GLN
1	A	870	GLN
1	A	882	HIS
1	A	904	HIS
1	A	927	HIS
1	A	932	GLN
1	A	959	ASN
1	B	58	ASN
1	B	106	GLN
1	B	145	HIS
1	B	147	GLN
1	B	159	HIS
1	B	169	GLN
1	B	272	HIS
1	B	294	ASN
1	B	419	ASN
1	B	489	ASN
1	B	544	GLN
1	B	598	ASN
1	B	624	ASN
1	B	651	HIS
1	B	721	ASN
1	B	763	HIS
1	B	811	GLN
1	B	860	HIS
1	B	869	GLN
1	B	870	GLN
1	B	882	HIS
1	B	904	HIS
1	B	927	HIS
1	B	932	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 ⓘ

8 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	1071	1,4	14,14,15	0.65	0	15,19,21	1.11	1 (6%)
4	NAG	A	1072	4	14,14,15	0.47	0	15,19,21	1.62	2 (13%)
4	NAG	A	1073	1,4	14,14,15	0.59	0	15,19,21	1.89	2 (13%)
4	NAG	A	1074	4	14,14,15	0.51	0	15,19,21	0.60	0
7	NAG	B	1077	1,7	14,14,15	0.45	0	15,19,21	1.59	3 (20%)
7	NAG	B	1078	7	14,14,15	0.56	0	15,19,21	1.42	2 (13%)
7	MAN	B	1079	7	11,11,12	0.69	0	14,15,17	1.03	0
7	MAN	B	1080	7	11,11,12	0.57	0	14,15,17	0.69	0

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	1071	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1072	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1073	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1074	4	-	0/6/23/26	0/1/1/1
7	NAG	B	1077	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1078	7	-	0/6/23/26	0/1/1/1
7	MAN	B	1079	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	B	1080	7	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1071	NAG	C2-N2-C7	-3.07	119.10	123.04
7	B	1077	NAG	C4-C3-C2	-2.90	106.72	111.23
4	A	1072	NAG	C2-N2-C7	-2.89	119.33	123.04
4	A	1073	NAG	C2-N2-C7	-2.10	120.35	123.04
7	B	1078	NAG	C6-C5-C4	-2.04	107.98	113.02
7	B	1077	NAG	C3-C2-N2	2.26	115.97	110.56
7	B	1077	NAG	C1-O5-C5	3.70	116.95	112.25
7	B	1078	NAG	C1-O5-C5	4.12	117.48	112.25
4	A	1072	NAG	C1-O5-C5	4.70	118.22	112.25
4	A	1073	NAG	C1-O5-C5	6.56	120.58	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1080	MAN	C1
7	B	1079	MAN	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	1071	NAG	3	0
4	A	1072	NAG	1	0
4	A	1073	NAG	2	0
4	A	1074	NAG	1	0
7	B	1079	MAN	1	0

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
5	NAG	A	1075	1	14,14,15	0.49	0	15,19,21	1.11	1 (6%)
5	NAG	A	1076	1	14,14,15	0.69	0	15,19,21	1.86	4 (26%)
6	MES	A	1083	-	11,12,12	0.83	0	14,16,16	2.54	6 (42%)
3	LYS	A	968	2	6,9,9	0.29	0	4,10,10	0.36	0
5	NAG	B	1081	1	14,14,15	0.68	0	15,19,21	0.85	0
6	MES	B	1084	-	11,12,12	0.70	0	14,16,16	2.72	8 (57%)
3	LYS	B	968	2	6,9,9	0.41	0	4,10,10	0.31	0

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
5	NAG	A	1075	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1076	1	-	0/6/23/26	0/1/1/1
6	MES	A	1083	-	-	0/6/14/14	0/1/1/1
3	LYS	A	968	2	-	0/5/9/9	0/0/0/0
5	NAG	B	1081	1	-	0/6/23/26	0/1/1/1
6	MES	B	1084	-	-	0/6/14/14	0/1/1/1
3	LYS	B	968	2	-	0/5/9/9	0/0/0/0

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1084	MES	C6-C5-N4	-4.44	103.39	110.12
5	A	1076	NAG	C2-N2-C7	-4.04	117.85	123.04
6	A	1083	MES	C6-C5-N4	-3.76	104.43	110.12
6	A	1083	MES	C2-C3-N4	-3.47	104.87	110.12
6	B	1084	MES	C2-C3-N4	-3.33	105.07	110.12
5	A	1076	NAG	C3-C2-N2	-3.22	102.84	110.56
6	B	1084	MES	O3S-S-O1S	-2.11	106.70	111.61
6	B	1084	MES	O2S-S-C8	2.30	108.86	106.91
5	A	1076	NAG	C4-C3-C2	2.91	115.76	111.23
6	A	1083	MES	O2S-S-C8	2.94	109.41	106.91
5	A	1076	NAG	C1-O5-C5	3.04	116.11	112.25
6	B	1084	MES	C7-N4-C3	3.47	120.17	111.27
6	A	1083	MES	C7-N4-C5	3.49	120.22	111.27
6	A	1083	MES	C7-N4-C3	3.50	120.24	111.27
6	B	1084	MES	O1S-S-C8	3.50	109.89	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1075	NAG	C1-O5-C5	3.51	116.70	112.25
6	B	1084	MES	C7-N4-C5	3.71	120.79	111.27
6	B	1084	MES	C5-N4-C3	4.68	119.04	108.90
6	A	1083	MES	C5-N4-C3	4.91	119.53	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1083	MES	2	0
3	A	968	LYS	1	0
5	B	1081	NAG	3	0
6	B	1084	MES	4	0
3	B	968	LYS	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	869/967 (89%)	-0.25	10 (1%) 81 63	26, 61, 108, 138	2 (0%)
1	B	859/967 (88%)	-0.11	31 (3%) 46 23	27, 63, 111, 139	0
All	All	1728/1934 (89%)	-0.18	41 (2%) 62 39	26, 62, 109, 139	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	VAL	4.1
1	B	617	LYS	4.1
1	B	596	SER	3.6
1	A	102	SER	3.6
1	B	102	SER	3.3
1	B	638	HIS	3.3
1	B	553	LYS	3.1
1	B	714	ASN	3.1
1	B	618	THR	3.0
1	B	558	SER	2.9
1	A	924	GLN	2.9
1	B	781	SER	2.9
1	B	155	LYS	2.8
1	B	923	ALA	2.7
1	B	61	ARG	2.7
1	A	613	ASP	2.7
1	B	653	LEU	2.6
1	A	927	HIS	2.6
1	B	779	GLU	2.5
1	B	926	SER	2.5
1	A	583	ARG	2.5
1	A	502	SER	2.4
1	A	560	ARG	2.4
1	B	532	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	924	GLN	2.4
1	B	776	GLN	2.3
1	B	135	LYS	2.2
1	B	728	GLN	2.2
1	A	530	GLU	2.2
1	B	554	GLN	2.2
1	B	615	PRO	2.2
1	B	597	SER	2.2
1	B	108	ILE	2.2
1	B	678	ASP	2.2
1	B	564	GLU	2.1
1	A	130	TYR	2.1
1	B	65	GLN	2.1
1	B	583	ARG	2.1
1	B	648	ASN	2.1
1	A	765	PRO	2.0
1	B	423	GLU	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	A	1073	14/15	0.89	0.33	4.01	44,63,69,71	0
7	NAG	B	1077	14/15	0.93	0.21	1.06	45,65,74,75	0
4	NAG	A	1071	14/15	0.94	0.20	0.64	43,58,70,72	0
4	NAG	A	1072	14/15	0.91	0.22	0.13	62,77,82,90	0
7	NAG	B	1078	14/15	0.89	0.23	-	57,74,91,95	0
7	MAN	B	1080	11/12	0.86	0.35	-	98,112,120,124	0
7	MAN	B	1079	11/12	0.82	0.33	-	94,102,111,115	0
4	NAG	A	1074	14/15	0.63	0.63	-	78,88,106,128	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	B	1081	14/15	0.88	0.37	5.71	53,72,97,99	0
5	NAG	A	1075	14/15	0.91	0.30	2.97	58,81,86,93	0
3	LYS	B	968	10/10	0.95	0.20	1.58	36,51,71,71	0
6	MES	B	1084	12/12	0.88	0.27	1.52	53,71,88,100	0
6	MES	A	1083	12/12	0.91	0.22	1.19	46,68,81,96	0
3	LYS	A	968	10/10	0.99	0.12	-1.41	32,39,51,51	0
2	ZN	A	5000	1/1	1.00	0.09	-2.87	31,31,31,31	0
2	ZN	B	6000	1/1	0.99	0.07	-4.66	36,36,36,36	0
5	NAG	A	1076	14/15	0.84	0.31	-	59,91,103,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.