



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 06:50 AM EST

PDB ID : 4JBS  
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2 in complex with PHOSPHINIC PSEUDOTRIPEPTIDE inhibitor.  
Authors : Saridakis, E.; Birtley, J.; Stratikos, E.; Mavridis, I.M.  
Deposited on : unknown  
Resolution : 2.79 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

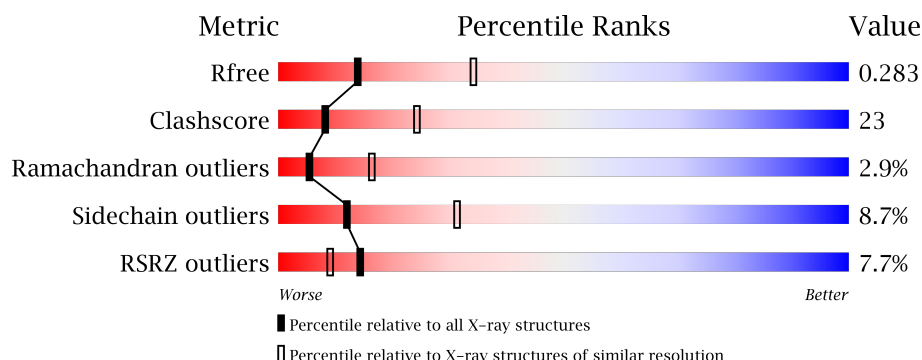
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3276 (2.80-2.76)
Clashscore	112137	3771 (2.80-2.76)
Ramachandran outliers	110173	3707 (2.80-2.76)
Sidechain outliers	110143	3709 (2.80-2.76)
RSRZ outliers	101464	3307 (2.80-2.76)

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>2%</div> <div>53%</div> <div>32%</div> <div>5%</div> <div>10%</div> </div>
1	B	967	<div> <div>12%</div> <div>43%</div> <div>41%</div> <div>5%</div> <div>12%</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	P52	A	1009	-	-	-	X
4	P52	B	1010	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14457 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
			7045	4547	1170	1301	27			
1	B	854	Total	C	N	O	S	0	0	0
			6831	4416	1130	1259	26			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q6P179
A	2	VAL	-	CLONING ARTIFACT	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	1	MET	-	CLONING ARTIFACT	UNP Q6P179
B	2	VAL	-	CLONING ARTIFACT	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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

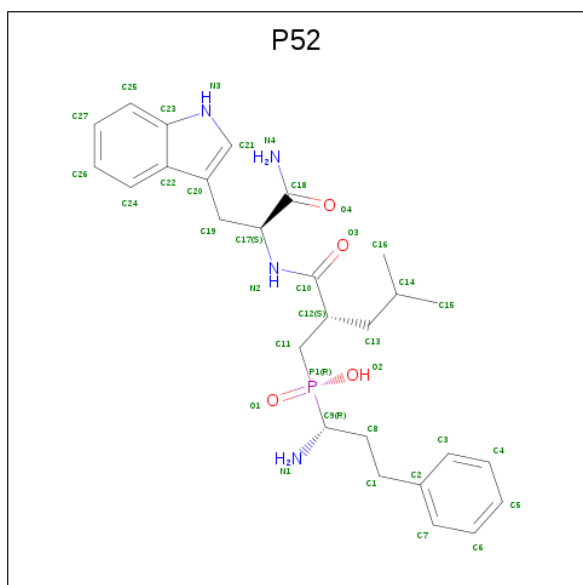


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

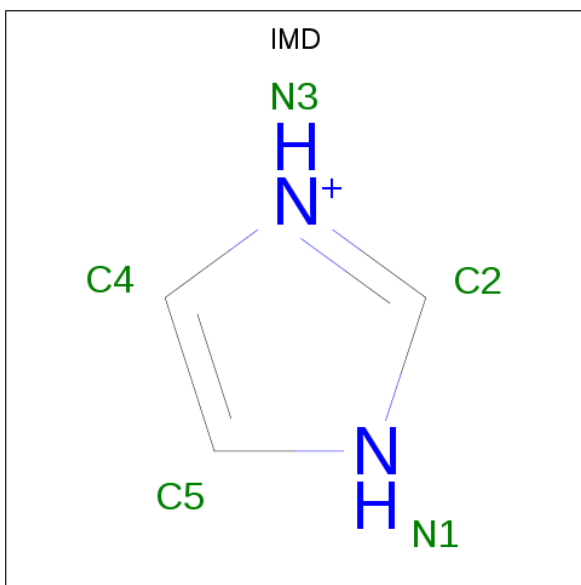
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is Nalpha-[(2S)-2-{[(1R)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]methyl}-4-methylpentanoyl]-L-tryptophanamide (three-letter code: P52) (formula: C<sub>27</sub>H<sub>37</sub>N<sub>4</sub>O<sub>4</sub>P).



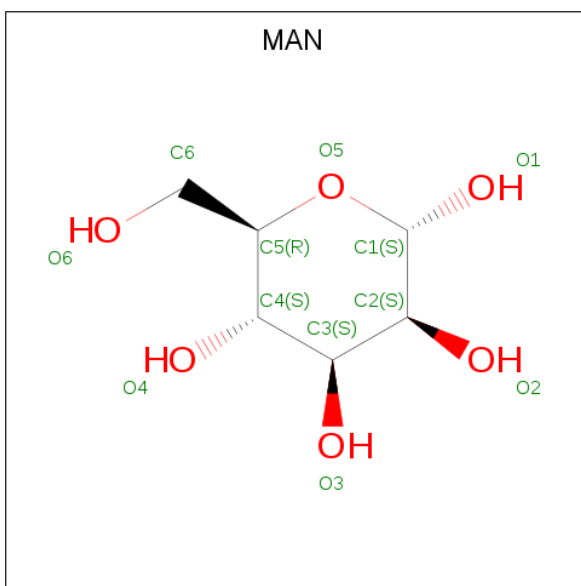
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	1	0
			36	27	4	4	1		
4	B	1	Total	C	N	O	P	1	0
			36	27	4	4	1		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



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

- Molecule 7 is water.

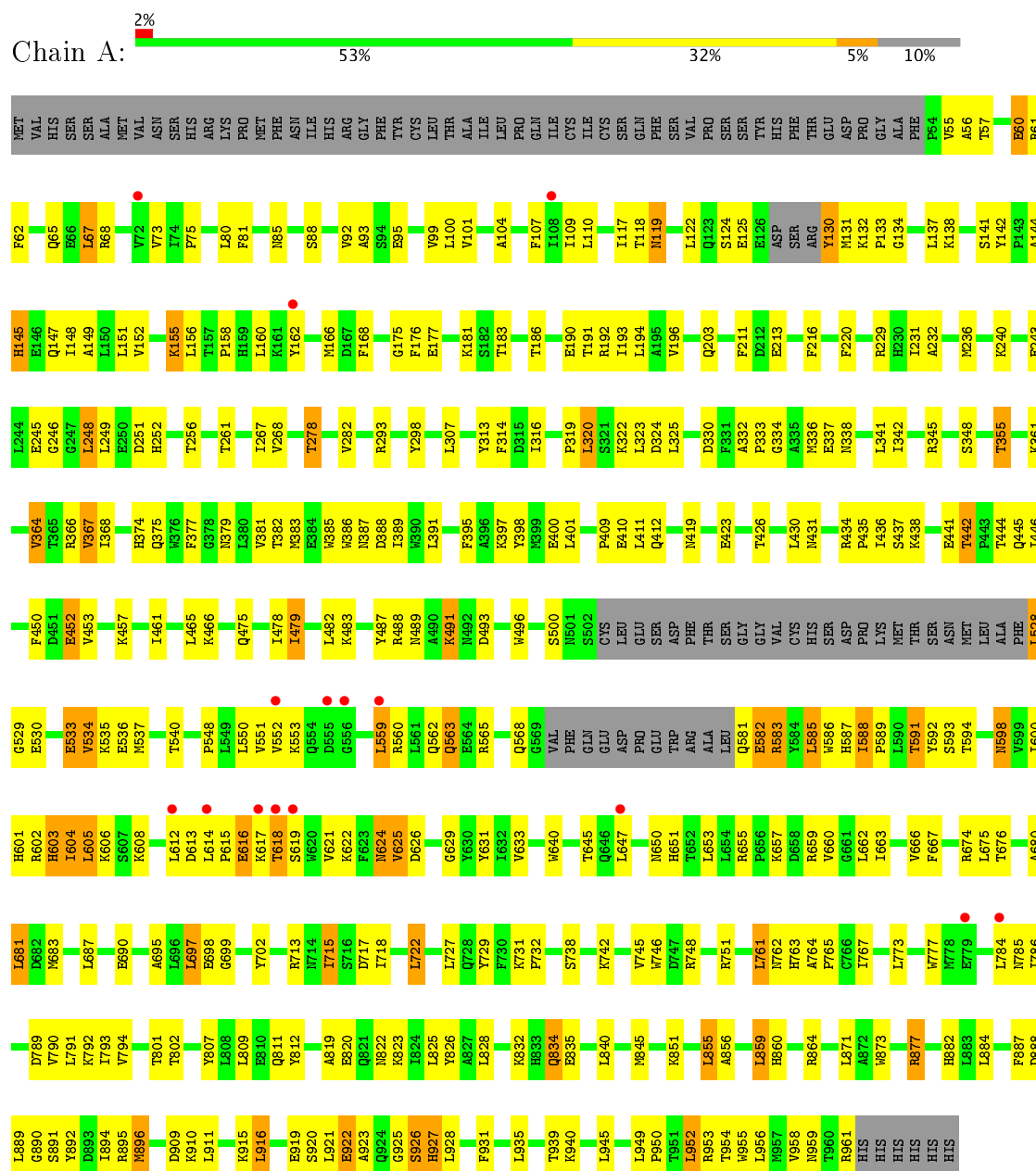
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	207	Total 207	O 207	0	0
7	B	86	Total 86	O 86	0	0



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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 2



- Molecule 1: Endoplasmic reticulum aminopeptidase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.15Å 134.77Å 128.73Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	10.99 – 2.79 48.77 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.7 (10.99-2.79) 99.8 (48.77-2.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.206 , 0.278 0.213 , 0.283	Depositor DCC
$R_{free}$ test set	3226 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 65.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.006 for -h,l,k 0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14457	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 3.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MAN, NAG, P52, IMD

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	0/7222	0.46	0/9787
1	B	0.26	0/6995	0.45	0/9488
All	All	0.27	0/14217	0.46	0/19275

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7045	0	6981	282	0
1	B	6831	0	6698	374	0
2	A	98	0	89	0	0
2	B	84	0	75	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	36	3	0
4	B	36	0	35	2	0
5	A	10	0	10	0	0
6	B	22	0	19	3	0
7	A	207	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	86	0	0	0	0
All	All	14457	0	13943	658	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 23.

All (658) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:HB1	1:A:57:THR:HA	1.31	1.09
1:B:374:HIS:HE1	1:B:392:LYS:HG2	1.29	0.96
1:B:565:ARG:HD2	1:B:584:TYR:HE2	1.28	0.94
1:B:582:GLU:N	1:B:583:ARG:HB2	1.85	0.92
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.50	0.91
1:B:889:LEU:HD21	1:B:925:GLY:HA2	1.55	0.89
1:A:122:LEU:HB2	1:A:137:LEU:HD21	1.55	0.87
1:B:784:LEU:HD22	1:B:785:ASN:H	1.39	0.87
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.58	0.86
1:B:355:THR:HG21	1:B:820:GLU:HB2	1.58	0.86
1:B:122:LEU:HB2	1:B:137:LEU:HD21	1.57	0.86
1:A:75:PRO:HG3	1:A:211:PHE:CD1	2.11	0.85
1:A:118:THR:O	1:A:119:ASN:HB2	1.75	0.84
1:A:56:ALA:CB	1:A:57:THR:HA	2.07	0.84
1:A:355:THR:HG21	1:A:820:GLU:HB2	1.60	0.83
1:B:374:HIS:CE1	1:B:392:LYS:HG2	2.12	0.83
1:B:104:ALA:H	1:B:158:PRO:HG3	1.43	0.82
1:A:528:LEU:HD23	1:A:529:GLY:HA2	1.59	0.82
1:A:591:THR:HB	1:A:625:VAL:HG23	1.60	0.82
1:B:565:ARG:HD2	1:B:584:TYR:CE2	2.14	0.81
1:B:712:ARG:HA	1:B:866:PRO:HG3	1.64	0.79
1:B:75:PRO:HG3	1:B:211:PHE:CD1	2.16	0.79
1:A:915:LYS:O	1:A:919:GLU:HG2	1.83	0.79
1:A:581:GLN:HG3	1:A:582:GLU:H	1.47	0.78
1:A:662:LEU:HB3	1:A:683:MET:HE1	1.65	0.78
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.18	0.78
1:A:152:VAL:HG21	1:A:156:LEU:HD21	1.64	0.77
1:B:777:TRP:HA	1:B:784:LEU:HB3	1.66	0.77
1:B:152:VAL:HG12	1:B:154:GLU:H	1.50	0.76
1:A:398:TYR:OH	1:A:466:LYS:HD3	1.87	0.75
1:B:911:LEU:O	1:B:915:LYS:HB2	1.87	0.75
1:A:537:MET:O	1:A:540:THR:HG22	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:TRP:CZ3	1:B:666:VAL:HG22	2.21	0.74
1:A:475:GLN:O	1:A:479:ILE:HG12	1.87	0.74
1:B:464:MET:HG3	1:B:629:GLY:HA2	1.70	0.74
1:B:411:LEU:HA	1:B:745:VAL:HG21	1.70	0.73
1:B:626:ASP:HA	1:B:657:LYS:HB3	1.70	0.73
1:B:56:ALA:HB2	1:B:62:PHE:N	2.04	0.73
1:B:338:ASN:HB2	1:B:341:LEU:O	1.89	0.73
1:A:56:ALA:HB1	1:A:57:THR:CA	2.15	0.72
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.70	0.72
1:B:877:ARG:HG3	1:B:917:PHE:CD1	2.24	0.72
1:A:245:GLU:HG2	1:A:246:GLY:H	1.54	0.72
1:B:69:LEU:HD13	1:B:211:PHE:HD2	1.55	0.71
1:A:935:LEU:O	1:A:939:THR:HG23	1.91	0.71
1:B:943:LYS:O	1:B:947:LYS:HB3	1.90	0.71
1:A:551:VAL:HB	1:A:562:GLN:HB2	1.73	0.70
1:B:843:LEU:HD22	1:B:849:VAL:HB	1.73	0.70
1:B:548:PRO:HG3	1:B:586:TRP:CG	2.27	0.70
1:B:889:LEU:HB3	1:B:894:ILE:HG21	1.73	0.70
1:B:632:ILE:HG22	1:B:633:VAL:H	1.57	0.69
1:A:366[B]:ARG:HH21	1:A:397:LYS:NZ	1.91	0.69
1:A:738:SER:O	1:A:751:ARG:HD3	1.92	0.69
6:B:1001:MAN:H3	6:B:1002:MAN:H2	1.75	0.68
1:B:540:THR:HG21	1:B:587:HIS:HB2	1.74	0.68
1:B:83:HIS:NE2	2:B:1003:NAG:H83	2.08	0.68
1:A:615:PRO:O	1:A:616:GLU:HG3	1.93	0.68
1:A:884:LEU:HD21	1:A:889:LEU:HD23	1.75	0.68
1:A:183:THR:HG22	1:A:193:ILE:HG12	1.76	0.68
1:B:843:LEU:O	1:B:846:GLU:HB3	1.93	0.68
1:A:533:GLU:HG2	1:A:536:GLU:HB2	1.76	0.67
1:A:191:THR:H	1:B:191:THR:HB	1.58	0.67
1:A:220:PHE:O	1:A:256:THR:HG23	1.94	0.67
1:B:947:LYS:HG3	1:B:947:LYS:O	1.94	0.67
1:B:442:THR:HG23	1:B:445:GLN:H	1.59	0.67
1:B:419:ASN:HD22	1:B:419:ASN:N	1.93	0.67
1:A:604:ILE:HG22	1:A:605:LEU:H	1.61	0.66
1:B:588:ILE:HG23	1:B:605:LEU:HD23	1.76	0.66
1:B:388:ASP:HB3	1:B:391:LEU:HG	1.76	0.66
1:B:62:PHE:CE1	1:B:142:TYR:HB2	2.31	0.65
1:B:62:PHE:CD1	1:B:142:TYR:HB2	2.31	0.65
1:B:674:ARG:HH11	1:B:674:ARG:HB3	1.61	0.65
1:B:313:TYR:HE2	1:B:478:ILE:HD11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.79	0.65
1:A:602:ARG:O	1:A:603:HIS:HB2	1.96	0.65
1:A:784:LEU:HD22	1:A:785:ASN:H	1.62	0.65
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.32	0.65
1:B:570:VAL:HB	1:B:943:LYS:HG3	1.78	0.65
1:B:536:GLU:O	1:B:540:THR:HG22	1.97	0.64
1:A:550:LEU:HB3	1:A:633:VAL:HG12	1.79	0.64
1:B:764:ALA:HB3	1:B:765:PRO:HD3	1.80	0.64
1:B:949:LEU:N	1:B:950:PRO:HD2	2.11	0.64
1:A:650:ASN:HB3	1:A:653:LEU:HG	1.79	0.64
1:B:152:VAL:HG21	1:B:156:LEU:HD21	1.80	0.64
1:A:355:THR:CG2	1:A:820:GLU:HB2	2.27	0.64
1:B:594:THR:HA	1:B:620:TRP:O	1.98	0.63
1:B:405:ASN:O	1:B:409:PRO:HG3	1.98	0.63
1:B:398:TYR:OH	1:B:466:LYS:HD3	1.98	0.63
1:B:245:GLU:CG	1:B:246:GLY:H	2.11	0.63
1:B:412:GLN:CD	1:B:746:TRP:HD1	2.02	0.63
1:B:310:TYR:HD1	1:B:314:PHE:CE2	2.16	0.63
1:B:922:GLU:OE1	1:B:922:GLU:HA	1.97	0.63
1:B:57:THR:HB	1:B:58:ASN:CG	2.19	0.63
1:B:431:ASN:HA	1:B:565:ARG:HH22	1.63	0.62
1:B:662:LEU:O	1:B:666:VAL:HG23	1.99	0.62
1:B:678:ASP:HA	1:B:681:LEU:HB2	1.81	0.62
1:B:635:TYR:HB2	1:B:640:TRP:CD1	2.34	0.62
1:B:626:ASP:HA	1:B:657:LYS:CB	2.29	0.62
1:B:767:ILE:O	1:B:767:ILE:HG13	1.98	0.62
1:A:666:VAL:HG21	1:A:683:MET:SD	2.39	0.62
1:B:582:GLU:N	1:B:583:ARG:CB	2.60	0.62
1:B:659:ARG:O	1:B:663:ILE:HG13	1.99	0.62
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.81	0.62
1:B:910:LYS:HD3	1:B:913:GLU:OE2	1.99	0.62
1:A:892:TYR:O	1:A:896:MET:HB3	2.00	0.61
1:A:568:GLN:HG2	1:A:940:LYS:HE2	1.82	0.61
1:B:731:LYS:N	1:B:732:PRO:HD2	2.15	0.61
1:B:906:SER:HB3	1:B:941:ASN:HB3	1.81	0.61
1:A:293:ARG:NH2	6:B:1001:MAN:O2	2.33	0.61
1:B:656:PRO:O	1:B:660:VAL:HG23	2.00	0.61
1:A:594:THR:HG22	1:A:621:VAL:HG12	1.82	0.61
1:A:911:LEU:O	1:A:915:LYS:HB2	2.00	0.61
1:B:802:THR:OG1	1:B:833:HIS:HE1	1.84	0.61
1:A:338:ASN:HB2	1:A:341:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TRP:HD1	1:A:387:ASN:HD22	1.45	0.61
1:B:565:ARG:O	1:B:567:LEU:HD12	2.01	0.61
1:A:727:LEU:HD21	1:A:761:LEU:HB3	1.82	0.60
1:B:666:VAL:HG21	1:B:683:MET:SD	2.41	0.60
6:B:1001:MAN:C3	6:B:1002:MAN:H2	2.31	0.60
1:B:604:ILE:HG22	1:B:605:LEU:H	1.66	0.60
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.81	0.60
1:A:382:THR:O	1:A:489:ASN:HA	2.01	0.60
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.81	0.60
1:B:330:ASP:OD1	1:B:851:LYS:HD2	2.00	0.60
1:B:488:ARG:HG2	1:B:489:ASN:H	1.66	0.60
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.84	0.60
1:B:236:MET:HG2	1:B:256:THR:HG22	1.83	0.60
1:B:664:HIS:O	1:B:668:GLN:HG2	2.02	0.60
1:A:213:GLU:HB2	1:A:216:PHE:CD2	2.37	0.60
1:A:581:GLN:HG3	1:A:582:GLU:N	2.17	0.59
1:B:791:LEU:HD11	1:B:795:TYR:CZ	2.36	0.59
1:A:314:PHE:O	1:A:316:ILE:HG13	2.02	0.59
1:A:582:GLU:O	1:A:583:ARG:CB	2.50	0.59
1:B:643:LEU:O	1:B:646:GLN:HB3	2.03	0.59
1:A:119:ASN:O	1:A:166:MET:HA	2.02	0.59
1:A:232:ALA:HB3	1:A:251:ASP:OD2	2.03	0.59
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.85	0.59
1:B:475:GLN:O	1:B:479:ILE:HG12	2.03	0.59
1:B:540:THR:HG21	1:B:587:HIS:H	1.68	0.59
1:B:626:ASP:HB3	1:B:657:LYS:HD3	1.85	0.59
1:A:533:GLU:HG2	1:A:533:GLU:O	2.01	0.58
1:B:140:LEU:HD12	1:B:151:LEU:HD11	1.85	0.58
1:A:450:PHE:O	1:A:895:ARG:NH2	2.36	0.58
1:A:500:SER:HB3	1:A:534:VAL:HB	1.85	0.58
1:A:186:THR:HG23	1:A:190:GLU:O	2.04	0.58
1:A:662:LEU:O	1:A:666:VAL:HG23	2.04	0.58
1:A:640:TRP:CD1	1:A:675:LEU:HD11	2.38	0.58
1:B:484:LYS:HD3	1:B:485:PHE:CZ	2.39	0.58
1:B:491:LYS:HG2	1:B:492:ASN:N	2.19	0.58
1:A:332:ALA:HB3	1:A:333:PRO:HD3	1.86	0.57
1:B:422:PHE:HA	1:B:425:ILE:HD12	1.85	0.57
1:B:468:PHE:CG	1:B:468:PHE:O	2.57	0.57
1:A:109:ILE:HD13	1:A:149:ALA:HA	1.87	0.57
1:B:56:ALA:O	1:B:57:THR:HG23	2.03	0.57
1:B:709:MET:O	1:B:713:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:PRO:HG3	1:A:586:TRP:CD2	2.39	0.57
1:B:310:TYR:CD1	1:B:314:PHE:HE2	2.23	0.57
1:B:310:TYR:O	1:B:314:PHE:HB2	2.05	0.57
1:B:419:ASN:HD22	1:B:419:ASN:H	1.51	0.57
1:B:731:LYS:N	1:B:732:PRO:CD	2.68	0.57
1:B:934:VAL:O	1:B:938:ILE:HG13	2.05	0.57
1:A:192:ARG:HA	1:B:190:GLU:HG2	1.86	0.57
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.20	0.57
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.87	0.56
1:A:856:ALA:HB1	1:A:896:MET:HG2	1.87	0.56
1:B:182:SER:OG	1:B:330:ASP:HB2	2.05	0.56
1:A:348:SER:HB3	1:A:367:VAL:HG21	1.87	0.56
1:B:245:GLU:CG	1:B:246:GLY:N	2.68	0.56
1:A:85:ASN:HB3	1:A:88:SER:HB3	1.85	0.56
1:B:236:MET:CE	1:B:256:THR:HA	2.35	0.56
1:B:566:PHE:CE2	1:B:672:ALA:HB2	2.40	0.56
1:B:954:THR:O	1:B:958:VAL:HG23	2.05	0.56
1:A:385:TRP:HD1	1:A:387:ASN:ND2	2.02	0.56
1:A:95:GLU:HG2	1:A:168:PHE:HE1	1.68	0.56
1:B:355:THR:CG2	1:B:820:GLU:HB2	2.34	0.56
1:B:568:GLN:NE2	1:B:671:GLY:HA3	2.21	0.56
1:B:846:GLU:HG3	1:B:848:LYS:H	1.71	0.56
1:A:141:SER:HA	1:A:148:ILE:HG22	1.86	0.56
1:A:240:LYS:HG2	1:A:252:HIS:HB2	1.88	0.56
1:A:475:GLN:HG2	1:A:479:ILE:HD11	1.86	0.56
1:B:245:GLU:CD	1:B:246:GLY:H	2.09	0.56
1:A:125:GLU:HA	1:A:125:GLU:OE1	2.06	0.56
1:A:320:LEU:HD23	1:A:320:LEU:N	2.21	0.56
2:B:1005:NAG:H61	2:B:1006:NAG:H83	1.86	0.55
1:B:63:PRO:HB2	1:B:107:PHE:CD1	2.40	0.55
1:B:468:PHE:CD2	1:B:469:LEU:HG	2.41	0.55
1:B:784:LEU:HD22	1:B:785:ASN:N	2.14	0.55
1:A:124:SER:HB2	1:A:131:MET:O	2.06	0.55
1:A:487:TYR:HA	7:A:1152:HOH:O	2.06	0.55
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.87	0.55
1:A:748:ARG:HB3	1:A:789:ASP:OD2	2.06	0.55
1:B:703:LEU:HD13	1:B:726:LEU:HD21	1.87	0.55
1:A:245:GLU:HG2	1:A:246:GLY:N	2.20	0.55
1:A:828:LEU:HD23	1:A:840:LEU:HD21	1.89	0.55
1:B:545:LYS:HG2	1:B:546:GLY:H	1.71	0.55
1:B:697:LEU:HD21	1:B:750:LEU:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:TYR:O	1:A:811[B]:GLN:HG2	2.07	0.55
1:B:318:TYR:CE2	1:B:323:LEU:HB2	2.42	0.55
1:B:731:LYS:HE3	1:B:763:HIS:CE1	2.40	0.55
1:B:777:TRP:CB	1:B:786:ILE:HD11	2.37	0.55
1:B:485:PHE:CZ	1:B:494:ASP:HB3	2.41	0.55
1:A:528:LEU:HD23	1:A:529:GLY:CA	2.35	0.55
1:B:655:ARG:HB2	1:B:658:ASP:OD2	2.07	0.55
1:A:625:VAL:HG12	1:A:655:ARG:HD2	1.87	0.55
1:B:422:PHE:O	1:B:425:ILE:HB	2.07	0.55
1:A:889:LEU:HB2	1:A:928:LEU:HD11	1.88	0.54
1:B:236:MET:HE2	1:B:256:THR:HG22	1.88	0.54
1:A:919:GLU:OE2	1:A:919:GLU:HA	2.06	0.54
1:B:729:TYR:C	1:B:731:LYS:H	2.11	0.54
1:B:889:LEU:HB2	1:B:928:LEU:HD11	1.89	0.54
1:A:784:LEU:HD13	1:A:785:ASN:N	2.23	0.54
1:B:374:HIS:CE1	1:B:392:LYS:CG	2.88	0.54
1:A:236:MET:HE2	1:A:256:THR:HA	1.89	0.54
1:B:58:ASN:ND2	1:B:58:ASN:N	2.55	0.54
1:A:548:PRO:HG3	1:A:586:TRP:CE3	2.43	0.54
1:A:834:GLN:H	1:A:834:GLN:HE21	1.55	0.54
1:A:528:LEU:CD2	1:A:529:GLY:HA2	2.33	0.54
1:B:442:THR:HG22	1:B:445:GLN:CD	2.28	0.54
1:A:100:LEU:HD12	1:A:101:VAL:N	2.22	0.54
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.43	0.54
1:B:298:TYR:CE2	1:B:361:LYS:HD2	2.43	0.54
1:B:540:THR:O	1:B:544:GLN:HG2	2.09	0.53
1:A:236:MET:CE	1:A:256:THR:HA	2.39	0.53
1:A:911:LEU:CD1	1:A:939:THR:HG22	2.37	0.53
1:B:227:GLU:OE1	1:B:229:ARG:HD3	2.09	0.53
1:B:272:HIS:CE1	1:B:290:PRO:HB3	2.44	0.53
1:A:381:VAL:HG21	1:A:482:LEU:HA	1.89	0.53
1:A:731:LYS:N	1:A:732:PRO:CD	2.72	0.53
1:A:764:ALA:HB3	1:A:765:PRO:HD3	1.89	0.53
1:B:659:ARG:HD2	1:B:690:GLU:OE1	2.08	0.53
1:A:156:LEU:HD12	1:A:162:TYR:CE1	2.44	0.53
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.44	0.53
1:B:245:GLU:HG2	1:B:246:GLY:H	1.72	0.53
1:B:56:ALA:HB2	1:B:62:PHE:H	1.74	0.53
1:B:702:TYR:O	1:B:705:SER:HB3	2.08	0.53
1:B:859:LEU:HD23	1:B:897:ILE:HG23	1.91	0.53
1:B:99:VAL:O	1:B:100:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:HA	1:B:413:PHE:CE2	2.44	0.53
1:B:622:LYS:HZ3	1:B:662:LEU:HG	1.72	0.53
1:B:718:ILE:HD11	1:B:952:LEU:HD13	1.91	0.53
1:B:960:THR:O	1:B:960:THR:HG22	2.08	0.53
1:B:559:LEU:O	1:B:611:THR:HG23	2.09	0.53
1:A:278:THR:CG2	1:A:282:VAL:HB	2.39	0.52
1:A:444:THR:HG23	1:A:890:GLY:H	1.73	0.52
1:A:475:GLN:O	1:A:478:ILE:HG12	2.09	0.52
1:B:145:HIS:O	1:B:147:GLN:HG3	2.10	0.52
1:B:245:GLU:HG2	1:B:246:GLY:N	2.23	0.52
1:B:381:VAL:HG13	1:B:485:PHE:HB2	1.91	0.52
1:B:173:GLY:H	1:B:180:TYR:HA	1.74	0.52
1:B:351:PHE:CZ	1:B:361:LYS:HE2	2.45	0.52
1:A:763:HIS:CD2	1:A:765:PRO:HD2	2.45	0.52
1:B:278:THR:HG22	1:B:304:LEU:HD23	1.92	0.52
1:B:384:GLU:HG3	1:B:490:ALA:O	2.09	0.52
1:A:366[B]:ARG:HG3	1:A:400:GLU:OE1	2.09	0.52
1:A:624:ASN:HD21	1:A:629:GLY:H	1.57	0.52
1:B:834:GLN:OE1	1:B:834:GLN:HA	2.09	0.52
1:A:559:LEU:HD12	1:A:612:LEU:O	2.10	0.52
1:A:922:GLU:HA	1:A:926:SER:HB2	1.92	0.52
1:B:173:GLY:N	1:B:180:TYR:HA	2.25	0.52
1:B:780:SER:O	1:B:783:LYS:HD3	2.10	0.52
1:A:889:LEU:HD12	1:A:889:LEU:O	2.09	0.51
1:B:67:LEU:HB3	1:B:145:HIS:CD2	2.44	0.51
1:B:916:LEU:O	1:B:916:LEU:HD13	2.10	0.51
1:B:935:LEU:O	1:B:939:THR:HG23	2.11	0.51
1:A:374:HIS:HA	1:A:377:PHE:O	2.10	0.51
1:B:731:LYS:HE3	1:B:763:HIS:HE1	1.74	0.51
1:A:722:LEU:HD13	1:A:956:LEU:HD11	1.91	0.51
1:B:857:ALA:HA	1:B:896:MET:HE1	1.92	0.51
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.92	0.51
1:A:624:ASN:HD21	1:A:629:GLY:N	2.09	0.51
1:B:465:LEU:HD12	1:B:468:PHE:HD2	1.76	0.51
1:B:568:GLN:O	1:B:569:GLY:O	2.28	0.51
1:B:905:PHE:O	1:B:938:ILE:HG23	2.10	0.51
1:A:388:ASP:HB3	1:A:391:LEU:CD1	2.41	0.51
1:B:605:LEU:HD12	1:B:606:LYS:H	1.76	0.51
1:A:528:LEU:CB	1:A:529:GLY:HA2	2.40	0.51
1:B:332:ALA:HB3	1:B:333:PRO:HD3	1.92	0.51
1:B:465:LEU:HD11	1:B:534:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.76	0.51
1:B:370:HIS:CG	4:B:1010:P52:H25	2.46	0.51
1:B:465:LEU:HD12	1:B:468:PHE:CD2	2.46	0.51
1:B:647:LEU:HA	1:B:651:HIS:HB3	1.92	0.51
1:A:366[B]:ARG:HH21	1:A:397:LYS:HZ2	1.58	0.50
1:A:99:VAL:HG12	1:A:100:LEU:N	2.26	0.50
1:B:80:LEU:HB3	1:B:222:ILE:HD13	1.93	0.50
1:B:808:LEU:HB2	1:B:828:LEU:HD11	1.93	0.50
1:B:912:GLN:NE2	1:B:915:LYS:HD3	2.25	0.50
1:B:955:TRP:O	1:B:958:VAL:HB	2.11	0.50
1:A:213:GLU:HB2	1:A:216:PHE:HD2	1.75	0.50
1:B:491:LYS:HG2	1:B:492:ASN:H	1.76	0.50
1:A:81:PHE:O	1:A:93:ALA:HB1	2.11	0.50
1:A:568:GLN:HG2	1:A:940:LYS:HG3	1.93	0.50
1:B:428:ASP:OD1	1:B:546:GLY:HA2	2.12	0.50
1:B:635:TYR:H	1:B:640:TRP:HE1	1.59	0.50
1:A:436:ILE:HD12	1:A:461:ILE:HD13	1.93	0.50
1:B:635:TYR:HB3	1:B:639:GLY:HA3	1.93	0.50
1:B:786:ILE:HB	1:B:791:LEU:HD13	1.92	0.50
1:B:911:LEU:HG	1:B:911:LEU:O	2.11	0.50
1:A:659:ARG:O	1:A:663:ILE:HG13	2.11	0.49
1:A:674:ARG:O	1:A:675:LEU:HD12	2.10	0.49
1:B:877:ARG:HG3	1:B:917:PHE:CE1	2.47	0.49
1:B:870:GLN:HE22	1:B:910:LYS:NZ	2.10	0.49
1:A:177:GLU:HB3	1:A:203:GLN:HG2	1.94	0.49
1:A:873:TRP:O	1:A:877:ARG:HB2	2.12	0.49
1:B:83:HIS:CE1	1:B:225:ARG:HD2	2.47	0.49
1:A:183:THR:HA	1:A:192:ARG:O	2.12	0.49
1:A:681:LEU:HD21	1:A:952:LEU:HD23	1.94	0.49
1:A:954:THR:O	1:A:958:VAL:HG23	2.13	0.49
1:B:337:GLU:HG3	1:B:374:HIS:HB3	1.93	0.49
1:B:57:THR:HB	1:B:58:ASN:OD1	2.13	0.49
1:B:727:LEU:O	1:B:731:LYS:HD3	2.13	0.49
1:B:849:VAL:HG12	1:B:850:ILE:HG13	1.94	0.49
1:A:873:TRP:CE2	1:A:877:ARG:HD3	2.47	0.49
1:A:718:ILE:HG21	1:A:952:LEU:HD13	1.93	0.49
1:A:323:LEU:HD12	1:A:324:ASP:N	2.27	0.49
1:A:559:LEU:CD1	1:A:612:LEU:HB3	2.43	0.49
1:B:179:PHE:CD1	1:B:197:THR:HG22	2.48	0.49
1:B:275:SER:HB3	1:B:283:LYS:HE2	1.95	0.49
1:B:725:TYR:O	1:B:729:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:893:ASP:O	1:B:897:ILE:HG13	2.12	0.49
1:A:67:LEU:HD12	1:A:68:ARG:N	2.27	0.48
1:A:887:PHE:HB2	1:A:894:ILE:HG12	1.94	0.48
1:B:386:TRP:HB3	1:B:446:ILE:HG23	1.94	0.48
1:A:622:LYS:HD3	1:A:662:LEU:HD21	1.95	0.48
1:A:793:ILE:HG13	7:A:1128:HOH:O	2.14	0.48
4:A:1009:P52:H11	4:A:1009:P52:H32	1.95	0.48
1:A:325:LEU:N	1:A:325:LEU:HD12	2.29	0.48
1:A:333:PRO:O	1:A:345:ARG:HD2	2.14	0.48
1:B:159:HIS:O	1:B:160:LEU:HD22	2.13	0.48
1:B:186:THR:HG21	1:B:192:ARG:NH1	2.28	0.48
1:B:385:TRP:CG	1:B:386:TRP:N	2.81	0.48
1:B:582:GLU:N	1:B:583:ARG:CA	2.76	0.48
1:B:55:VAL:O	1:B:56:ALA:HB2	2.13	0.48
1:B:647:LEU:HD22	1:B:686:TYR:CE1	2.48	0.48
1:A:537:MET:CE	1:A:589:PRO:HG3	2.44	0.48
1:A:604:ILE:N	1:A:604:ILE:HD12	2.28	0.48
1:A:67:LEU:HB3	1:A:145:HIS:CD2	2.48	0.48
1:B:390:TRP:CG	1:B:436:ILE:HG23	2.48	0.48
1:B:660:VAL:HG22	1:B:695:ALA:CA	2.44	0.48
1:B:730:PHE:C	1:B:732:PRO:HD2	2.34	0.48
1:B:333:PRO:O	1:B:345:ARG:HD2	2.13	0.48
1:A:386:TRP:HB3	1:A:446:ILE:HG23	1.95	0.48
1:A:626:ASP:OD1	1:A:657:LYS:HB2	2.13	0.48
1:B:236:MET:HE2	1:B:256:THR:HA	1.94	0.48
1:B:889:LEU:HA	1:B:890:GLY:HA2	1.59	0.48
1:B:887:PHE:HB2	1:B:894:ILE:HG12	1.94	0.48
1:A:430:LEU:HD21	1:A:940:LYS:HE3	1.94	0.48
1:A:465:LEU:HD22	1:A:496:TRP:HZ3	1.79	0.48
1:B:364:VAL:O	1:B:368:ILE:HG13	2.14	0.48
1:A:659:ARG:HD2	1:A:690:GLU:OE1	2.13	0.48
1:B:738:SER:O	1:B:740:SER:N	2.45	0.48
1:A:731:LYS:N	1:A:732:PRO:HD2	2.29	0.47
1:A:834:GLN:HG3	1:A:871:LEU:HD12	1.95	0.47
1:B:248:LEU:O	1:B:249:LEU:HD23	2.14	0.47
1:B:352:ASP:OD2	1:B:355:THR:HB	2.14	0.47
1:B:622:LYS:NZ	1:B:662:LEU:HG	2.28	0.47
1:B:309:PHE:C	1:B:309:PHE:CD2	2.87	0.47
1:B:666:VAL:HG12	1:B:680:ALA:HB2	1.94	0.47
1:B:236:MET:HB3	1:B:254:GLU:HB3	1.95	0.47
1:A:375:GLN:O	1:A:379:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LEU:HB3	1:A:955:TRP:NE1	2.29	0.47
1:B:156:LEU:HD12	1:B:162:TYR:CE1	2.49	0.47
1:B:436:ILE:HD11	1:B:458:GLY:HA2	1.95	0.47
1:B:857:ALA:HA	1:B:896:MET:CE	2.44	0.47
1:A:533:GLU:O	1:A:535:LYS:N	2.48	0.47
1:B:540:THR:OG1	1:B:586:TRP:HA	2.14	0.47
1:B:614:LEU:C	1:B:616:GLU:H	2.17	0.47
1:B:918:PHE:CD1	1:B:918:PHE:N	2.82	0.47
1:A:479:ILE:HG22	1:A:483:LYS:HE3	1.97	0.47
1:B:100:LEU:HD13	1:B:161:LYS:HG2	1.97	0.47
1:B:902:THR:OG1	1:B:934:VAL:HG11	2.15	0.47
1:B:798:GLY:O	1:B:801:THR:HG22	2.15	0.47
1:A:330:ASP:OD1	1:A:851:LYS:HD2	2.15	0.47
1:B:278:THR:HG21	1:B:307:LEU:HD23	1.96	0.47
1:B:99:VAL:HG12	1:B:100:LEU:H	1.80	0.47
1:A:616:GLU:O	1:A:618:THR:N	2.49	0.46
1:A:889:LEU:HA	1:A:890:GLY:HA2	1.50	0.46
1:A:124:SER:HA	7:A:1231:HOH:O	2.15	0.46
1:A:388:ASP:HB3	1:A:391:LEU:HD12	1.97	0.46
1:B:582:GLU:CA	1:B:583:ARG:HB2	2.44	0.46
1:B:718:ILE:HG13	1:B:956:LEU:HD12	1.97	0.46
1:B:257:VAL:HB	2:B:1005:NAG:O6	2.15	0.46
1:B:332:ALA:O	1:B:345:ARG:NH1	2.48	0.46
1:B:588:ILE:O	1:B:605:LEU:HB3	2.14	0.46
1:B:870:GLN:HE22	1:B:910:LYS:HE3	1.80	0.46
1:A:488:ARG:HG2	1:A:489:ASN:N	2.30	0.46
1:B:467:ASP:CG	1:B:602:ARG:HH12	2.19	0.46
1:B:647:LEU:HD13	1:B:686:TYR:CD2	2.51	0.46
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.96	0.46
1:B:828:LEU:HB3	1:B:840:LEU:HD11	1.96	0.46
1:A:919:GLU:O	1:A:920:SER:C	2.54	0.46
1:B:703:LEU:CD1	1:B:726:LEU:HD21	2.45	0.46
1:A:118:THR:O	1:A:119:ASN:CB	2.53	0.46
1:A:647:LEU:O	1:A:651:HIS:HB3	2.16	0.46
1:B:310:TYR:OH	1:B:373:ALA:HB2	2.15	0.46
1:B:58:ASN:N	1:B:58:ASN:HD22	2.14	0.46
1:A:313:TYR:CE2	1:A:478:ILE:HD11	2.51	0.46
1:A:412:GLN:HB3	1:A:746:TRP:HE1	1.80	0.46
1:B:123:GLN:HG2	1:B:134:GLY:HA3	1.98	0.46
1:B:310:TYR:CD1	1:B:314:PHE:CE2	2.96	0.46
1:A:107:PHE:HB3	1:A:151:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LYS:HB3	1:A:560:ARG:HB2	1.98	0.46
1:B:442:THR:HG22	1:B:445:GLN:CG	2.46	0.46
1:B:674:ARG:O	1:B:675:LEU:HD12	2.15	0.46
1:A:786:ILE:CG2	1:A:790:VAL:HG23	2.46	0.46
1:A:409:PRO:HD2	1:A:410:GLU:OE2	2.16	0.45
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.98	0.45
1:B:186:THR:HG23	1:B:190:GLU:O	2.16	0.45
1:B:651:HIS:HD2	1:B:659:ARG:NH1	2.14	0.45
1:A:236:MET:HE1	1:A:320:LEU:HD22	1.98	0.45
1:B:119:ASN:O	1:B:166:MET:HA	2.16	0.45
1:B:537:MET:HA	1:B:587:HIS:CB	2.46	0.45
1:A:191:THR:HB	1:B:191:THR:H	1.82	0.45
1:A:959:ASN:C	1:A:961:ARG:H	2.19	0.45
1:B:375:GLN:O	1:B:379:ASN:HB2	2.16	0.45
1:B:873:TRP:CE3	1:B:873:TRP:HA	2.52	0.45
1:A:366[B]:ARG:HH21	1:A:397:LYS:HZ1	1.64	0.45
1:A:479:ILE:O	1:A:483:LYS:HG3	2.16	0.45
1:B:751:ARG:HG3	1:B:755:LEU:HD12	1.98	0.45
4:A:1009:P52:H26	4:A:1009:P52:H17	1.71	0.45
1:A:267:ILE:HD12	1:A:341:LEU:HD21	1.99	0.45
1:B:77:HIS:HD1	1:B:219:ASN:HB2	1.81	0.45
1:B:445:GLN:O	1:B:449:MET:HG2	2.16	0.45
1:B:535:LYS:O	1:B:538:MET:N	2.48	0.45
1:B:569:GLY:HA2	1:B:570:VAL:HA	1.69	0.45
1:B:707:TYR:HE1	1:B:723:LYS:HB2	1.81	0.45
1:A:592:TYR:CZ	1:A:601:HIS:HB2	2.52	0.45
1:B:729:TYR:HD2	1:B:730:PHE:N	2.15	0.45
1:A:145:HIS:O	1:A:147:GLN:HG3	2.17	0.45
1:A:411:LEU:HA	1:A:745:VAL:HG21	1.99	0.45
1:A:598:ASN:ND2	1:A:598:ASN:H	2.15	0.45
1:B:258:LYS:HG2	2:B:1005:NAG:O5	2.16	0.45
1:B:729:TYR:C	1:B:731:LYS:N	2.70	0.45
1:B:729:TYR:CD2	1:B:730:PHE:N	2.84	0.45
1:A:598:ASN:ND2	1:A:598:ASN:N	2.64	0.45
1:A:412:GLN:HB3	1:A:746:TRP:NE1	2.32	0.45
1:B:183:THR:HA	1:B:192:ARG:O	2.17	0.45
1:B:200:GLU:HA	1:B:201:PRO:HA	1.73	0.45
1:B:104:ALA:HB1	1:B:155:LYS:HD2	1.98	0.45
1:B:624:ASN:HA	1:B:624:ASN:HD22	1.59	0.45
1:A:452:GLU:HG2	1:A:452:GLU:H	1.32	0.45
1:A:68:ARG:HD3	7:A:1114:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ILE:HB	1:A:791:LEU:HD13	1.99	0.45
1:B:453:VAL:O	1:B:457:LYS:HB3	2.16	0.45
1:B:537:MET:O	1:B:541:TRP:CD1	2.70	0.45
1:B:718:ILE:HG13	1:B:956:LEU:CD1	2.47	0.45
1:A:156:LEU:HD12	1:A:162:TYR:CZ	2.52	0.44
1:A:434:ARG:NH1	1:A:435:PRO:O	2.50	0.44
1:A:598:ASN:N	1:A:598:ASN:HD22	2.13	0.44
1:A:916:LEU:HD22	1:A:916:LEU:HA	1.76	0.44
1:A:925:GLY:O	1:A:926:SER:C	2.54	0.44
1:B:342:ILE:HG22	1:B:344:TYR:CE1	2.51	0.44
1:A:809:LEU:O	1:A:812:TYR:HB3	2.17	0.44
1:B:273:SER:HB3	1:B:287:TYR:CD1	2.52	0.44
1:B:724:ARG:HB3	1:B:728:GLN:NE2	2.33	0.44
1:B:873:TRP:HE3	1:B:873:TRP:HA	1.82	0.44
1:A:624:ASN:HB2	1:A:631:TYR:CE2	2.53	0.44
1:A:860:HIS:CD2	1:A:864:ARG:HD2	2.52	0.44
1:A:926:SER:HA	1:A:927:HIS:HA	1.69	0.44
1:B:156:LEU:HD12	1:B:162:TYR:CZ	2.52	0.44
1:B:374:HIS:HA	1:B:377:PHE:O	2.18	0.44
1:B:774:PHE:CG	1:B:798:GLY:HA3	2.53	0.44
1:A:181:LYS:HE2	1:A:181:LYS:HB3	1.59	0.44
1:A:559:LEU:HD12	1:A:612:LEU:HB3	2.00	0.44
1:B:378:GLY:HA3	1:B:392:LYS:HG3	2.00	0.44
1:B:538:MET:O	1:B:541:TRP:HB2	2.17	0.44
1:B:588:ILE:HG12	1:B:588:ILE:O	2.16	0.44
1:B:651:HIS:HD2	1:B:659:ARG:HH11	1.65	0.44
1:B:75:PRO:HG2	1:B:216:PHE:HB3	2.00	0.44
1:A:553:LYS:O	1:A:559:LEU:HA	2.18	0.44
1:A:604:ILE:H	1:A:604:ILE:HD12	1.83	0.44
1:A:738:SER:O	1:A:751:ARG:CD	2.63	0.44
1:A:921:LEU:HD12	1:A:931:PHE:CZ	2.53	0.44
1:B:150:LEU:HD13	1:B:164:VAL:HG11	2.00	0.44
1:B:457:LYS:O	1:B:461:ILE:HG23	2.18	0.44
1:A:366[B]:ARG:NH2	1:A:397:LYS:NZ	2.64	0.44
1:A:600:ILE:HG23	1:A:625:VAL:HG21	1.99	0.44
1:A:651:HIS:C	1:A:651:HIS:CD2	2.91	0.44
1:A:660:VAL:HG22	1:A:695:ALA:HA	1.99	0.44
1:A:75:PRO:HG3	1:A:211:PHE:CG	2.52	0.44
1:B:117:ILE:HD13	1:B:166:MET:SD	2.58	0.44
1:B:421:CYS:O	1:B:425:ILE:HG13	2.18	0.44
1:B:217:LYS:HE3	1:B:489:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:HIS:CE1	1:B:689:HIS:HB3	2.52	0.44
1:B:832:LYS:HD3	1:B:832:LYS:HA	1.83	0.44
1:A:533:GLU:O	1:A:534:VAL:C	2.56	0.44
1:B:214:PRO:HA	1:B:260:SER:HB3	1.98	0.44
1:B:431:ASN:CA	1:B:565:ARG:HH22	2.29	0.44
1:B:927:HIS:O	1:B:928:LEU:HD23	2.18	0.44
1:B:931:PHE:O	1:B:935:LEU:HG	2.18	0.44
1:A:278:THR:HG23	1:A:282:VAL:HB	2.00	0.43
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.99	0.43
1:B:666:VAL:O	1:B:670:VAL:HG23	2.18	0.43
1:B:676:THR:HG23	1:B:679:LYS:H	1.83	0.43
1:B:729:TYR:O	1:B:731:LYS:N	2.51	0.43
1:B:96:LYS:HB3	1:B:96:LYS:HE3	1.77	0.43
1:B:624:ASN:HD21	1:B:629:GLY:N	2.15	0.43
1:B:713:ARG:HB2	1:B:715:ILE:HG13	1.99	0.43
1:A:366[B]:ARG:NH2	1:A:397:LYS:HZ2	2.15	0.43
1:B:357:SER:H	1:B:360:ASP:HB2	1.83	0.43
1:B:790:VAL:O	1:B:794:VAL:HG23	2.19	0.43
1:B:942:ILE:O	1:B:946:GLU:HG2	2.17	0.43
1:A:434:ARG:HD2	1:A:438:LYS:HD3	1.99	0.43
1:A:442:THR:HG22	1:A:445:GLN:CD	2.39	0.43
1:A:819:ALA:O	1:A:822:ASN:HB3	2.18	0.43
1:B:418:LEU:HA	1:B:418:LEU:HD23	1.88	0.43
1:A:104:ALA:HB1	1:A:155:LYS:HE2	2.00	0.43
1:A:488:ARG:CG	1:A:489:ASN:N	2.81	0.43
1:A:592:TYR:CE1	1:A:601:HIS:HB2	2.53	0.43
1:A:559:LEU:HD12	1:A:612:LEU:C	2.39	0.43
1:B:67:LEU:HB3	1:B:145:HIS:NE2	2.32	0.43
1:B:176:PHE:CD2	1:B:332:ALA:HB2	2.54	0.43
1:B:285:SER:O	1:B:286:ILE:HD13	2.18	0.43
1:B:419:ASN:ND2	1:B:419:ASN:N	2.64	0.43
1:A:386:TRP:CE3	1:A:389:ILE:HD13	2.53	0.43
1:A:792:LYS:HD3	1:A:826:TYR:CD2	2.54	0.43
1:B:95:GLU:HG2	1:B:168:PHE:HE1	1.83	0.43
1:B:479:ILE:O	1:B:483:LYS:HB2	2.18	0.43
1:A:57:THR:HG23	1:A:141:SER:O	2.18	0.43
1:B:78:TYR:HB2	1:B:220:PHE:CD1	2.54	0.43
1:B:545:LYS:CG	1:B:546:GLY:H	2.31	0.43
1:B:545:LYS:HG2	1:B:546:GLY:N	2.33	0.43
1:B:595:SER:HB3	1:B:620:TRP:CE2	2.53	0.43
1:B:647:LEU:HD23	1:B:651:HIS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:O	1:B:95:GLU:HA	2.19	0.43
1:A:832:LYS:HA	1:A:832:LYS:HD3	1.88	0.43
1:B:545:LYS:CG	1:B:546:GLY:N	2.81	0.43
1:B:860:HIS:C	1:B:860:HIS:CD2	2.92	0.43
1:B:724:ARG:HD2	1:B:728:GLN:HE22	1.84	0.43
1:B:797:VAL:O	1:B:800:GLN:HG2	2.19	0.43
1:A:565:ARG:HD3	1:A:581:GLN:HB2	2.00	0.42
1:A:587:HIS:HA	1:A:605:LEU:O	2.19	0.42
1:A:60:GLU:HB3	1:A:61:ARG:H	1.68	0.42
1:B:597:SER:C	1:B:599:VAL:H	2.22	0.42
1:B:624:ASN:CG	1:B:627:SER:HA	2.40	0.42
1:B:870:GLN:HE22	1:B:910:LYS:CE	2.31	0.42
1:A:142:TYR:CE1	1:A:144:ALA:HB3	2.54	0.42
1:A:364:VAL:O	1:A:368:ILE:HG13	2.19	0.42
1:A:873:TRP:CE3	1:A:873:TRP:HA	2.54	0.42
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.82	0.42
1:A:336:MET:O	1:A:342:ILE:HG23	2.18	0.42
1:A:298:TYR:CE2	1:A:361:LYS:HE3	2.54	0.42
1:B:595:SER:HA	1:B:620:TRP:CH2	2.54	0.42
1:B:866:PRO:O	1:B:869:GLN:HG2	2.18	0.42
1:A:457:LYS:O	1:A:461:ILE:HG23	2.19	0.42
1:A:945:LEU:O	1:A:949:LEU:HB2	2.20	0.42
1:B:154:GLU:O	1:B:155:LYS:C	2.58	0.42
1:B:214:PRO:HG3	1:B:386:TRP:CZ2	2.54	0.42
1:B:233:LEU:O	1:B:266:TYR:HA	2.19	0.42
1:B:604:ILE:H	1:B:604:ILE:HD12	1.84	0.42
1:B:695:ALA:HA	1:B:698:GLU:HB3	2.01	0.42
1:A:176:PHE:HE1	1:A:330:ASP:HB3	1.84	0.42
1:A:608:LYS:HD3	1:A:608:LYS:O	2.20	0.42
1:A:888:ASP:HB2	1:A:891:SER:HB3	2.02	0.42
1:B:777:TRP:HB2	1:B:784:LEU:HD12	2.01	0.42
1:A:130:TYR:HB3	1:A:131:MET:H	1.61	0.42
1:A:786:ILE:HG12	1:A:794:VAL:HG11	2.02	0.42
1:B:122:LEU:CB	1:B:137:LEU:HD21	2.39	0.42
1:B:181:LYS:HE2	1:B:181:LYS:HB3	1.80	0.42
1:B:248:LEU:C	1:B:249:LEU:HD23	2.40	0.42
1:B:949:LEU:N	1:B:950:PRO:CD	2.80	0.42
1:A:348:SER:O	1:A:364:VAL:HB	2.18	0.42
1:A:441:GLU:HB2	1:A:445:GLN:OE1	2.19	0.42
1:A:533:GLU:CG	1:A:533:GLU:O	2.66	0.42
1:A:581:GLN:CG	1:A:582:GLU:H	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ILE:HA	1:A:589:PRO:HD3	1.83	0.42
1:A:845:MET:SD	1:A:855:LEU:HD11	2.59	0.42
1:B:334:GLY:HA2	1:B:345:ARG:HD3	2.02	0.42
1:B:438:LYS:HG2	1:B:439:PRO:N	2.33	0.42
1:B:380:LEU:HD11	1:B:487:TYR:CE2	2.55	0.42
1:B:906:SER:CB	1:B:941:ASN:HB3	2.47	0.42
1:A:436:ILE:HA	1:A:453:VAL:HG12	2.01	0.42
1:B:429:SER:O	1:B:430:LEU:HD23	2.19	0.42
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.91	0.42
1:A:614:LEU:HA	1:A:615:PRO:HD3	1.87	0.42
1:A:855:LEU:HD22	1:A:859:LEU:HD22	2.02	0.42
1:B:324:ASP:C	1:B:325:LEU:HD12	2.39	0.42
1:B:436:ILE:CD1	1:B:458:GLY:HA2	2.50	0.42
1:B:647:LEU:O	1:B:651:HIS:HB3	2.20	0.42
1:B:726:LEU:O	1:B:729:TYR:O	2.38	0.42
1:B:943:LYS:HD3	1:B:943:LYS:HA	1.71	0.42
1:A:364:VAL:HA	1:A:367:VAL:HG13	2.00	0.42
1:A:488:ARG:CG	1:A:489:ASN:H	2.32	0.42
1:A:667:PHE:CE1	1:A:680:ALA:HB1	2.55	0.42
1:A:681:LEU:HD12	1:A:681:LEU:HA	1.84	0.42
1:B:270:ASP:OD1	1:B:270:ASP:N	2.53	0.42
1:B:469:LEU:O	1:B:473:LYS:HB3	2.20	0.42
1:B:710:MET:O	1:B:713:ARG:O	2.37	0.42
1:A:132:LYS:O	1:A:134:GLY:HA2	2.19	0.41
1:A:231:ILE:O	1:A:268:VAL:HA	2.20	0.41
1:A:588:ILE:HG12	1:A:588:ILE:O	2.20	0.41
1:A:604:ILE:O	1:A:605:LEU:HB2	2.20	0.41
1:A:717:ASP:OD1	1:A:953:ARG:NH1	2.53	0.41
1:B:444:THR:HG23	1:B:890:GLY:H	1.85	0.41
1:A:666:VAL:HG11	1:A:680:ALA:HA	2.01	0.41
1:B:408:TYR:N	1:B:409:PRO:HD3	2.35	0.41
1:B:314:PHE:O	1:B:316:ILE:HG13	2.19	0.41
1:B:770:ALA:HB1	1:B:797:VAL:HG21	2.03	0.41
1:A:117:ILE:CD1	1:A:148:ILE:HD13	2.51	0.41
1:A:479:ILE:H	1:A:479:ILE:HG12	1.64	0.41
1:A:884:LEU:HD12	1:A:884:LEU:HA	1.74	0.41
1:B:832:LYS:HB3	1:B:867:LYS:HE3	2.02	0.41
1:A:959:ASN:C	1:A:961:ARG:N	2.74	0.41
1:A:125:GLU:N	7:A:1231:HOH:O	2.51	0.41
1:A:950:PRO:HG2	7:A:1261:HOH:O	2.21	0.41
1:B:488:ARG:HG2	1:B:489:ASN:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ILE:HA	1:B:548:PRO:HD3	1.81	0.41
1:B:559:LEU:HD12	1:B:612:LEU:O	2.21	0.41
1:B:56:ALA:HB2	1:B:62:PHE:HB2	2.03	0.41
1:B:918:PHE:N	1:B:918:PHE:HD1	2.19	0.41
1:B:382:THR:HB	1:B:489:ASN:OD1	2.21	0.41
1:B:682:ASP:OD1	1:B:955:TRP:NE1	2.47	0.41
1:B:866:PRO:HA	1:B:869:GLN:OE1	2.20	0.41
1:B:888:ASP:O	1:B:891:SER:N	2.53	0.41
1:B:93:ALA:HB3	1:B:168:PHE:CE2	2.56	0.41
1:A:625:VAL:CG1	1:A:655:ARG:HD2	2.51	0.41
1:A:819:ALA:O	1:A:823:LYS:HG3	2.21	0.41
1:B:534:VAL:HG12	1:B:538:MET:HG2	2.03	0.41
1:B:924:GLN:C	1:B:926:SER:H	2.24	0.41
1:A:137:LEU:HD11	1:A:152:VAL:HG22	2.02	0.41
1:A:491:LYS:HE3	1:A:491:LYS:HB2	1.94	0.41
1:A:605:LEU:HD12	1:A:606:LYS:N	2.36	0.41
1:B:239:VAL:HG12	1:B:240:LYS:N	2.36	0.41
1:B:62:PHE:HA	1:B:63:PRO:HD3	1.68	0.41
1:B:918:PHE:HE2	1:B:934:VAL:HB	1.85	0.41
1:A:334:GLY:H	4:A:1009:P52:H18	1.68	0.41
1:B:707:TYR:CE1	1:B:723:LYS:HB2	2.56	0.41
1:A:385:TRP:CD1	1:A:387:ASN:ND2	2.85	0.40
1:A:910:LYS:HA	1:A:910:LYS:HD3	1.84	0.40
1:A:921:LEU:O	1:A:926:SER:OG	2.28	0.40
4:B:1010:P52:H27	4:B:1010:P52:H17	1.87	0.40
1:B:239:VAL:HG12	1:B:240:LYS:HD2	2.03	0.40
1:B:465:LEU:CD1	1:B:534:VAL:HG11	2.51	0.40
1:A:191:THR:O	1:B:190:GLU:HG2	2.21	0.40
1:A:412:GLN:NE2	1:A:745:VAL:HB	2.36	0.40
1:A:419:ASN:O	1:A:423:GLU:HG3	2.20	0.40
1:A:826:TYR:C	1:A:826:TYR:CD2	2.94	0.40
1:B:604:ILE:O	1:B:605:LEU:HB2	2.21	0.40
1:B:677:LEU:HG	1:B:681:LEU:HD22	2.04	0.40
1:B:82:VAL:O	1:B:84:PRO:HD3	2.21	0.40
1:B:838:LEU:HD22	1:B:838:LEU:O	2.21	0.40
1:B:865:ARG:HG2	1:B:865:ARG:H	1.65	0.40
1:A:248:LEU:O	1:A:249:LEU:HD23	2.20	0.40
1:A:614:LEU:HD12	1:A:615:PRO:HD2	2.02	0.40
1:A:698:GLU:OE2	1:A:702:TYR:HE2	2.03	0.40
1:A:715:ILE:HG21	1:A:718:ILE:HD12	2.02	0.40
1:B:103:ASN:O	1:B:104:ALA:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:THR:HG21	1:B:820:GLU:CB	2.41	0.40
1:B:537:MET:HA	1:B:587:HIS:HB2	2.02	0.40
1:B:74:ILE:HA	1:B:75:PRO:HD3	1.64	0.40
1:A:563:GLN:OE1	1:A:585:LEU:HA	2.22	0.40
1:A:882:HIS:O	1:A:882:HIS:ND1	2.54	0.40
1:B:197:THR:HB	1:B:199:PHE:CZ	2.57	0.40
1:B:757:LEU:O	1:B:761:LEU:HD22	2.21	0.40
1:B:898:ILE:HG22	1:B:899:SER:N	2.36	0.40
1:A:697:LEU:HD12	1:A:697:LEU:HA	1.84	0.40
1:B:78:TYR:CD2	1:B:220:PHE:CE1	3.09	0.40
1:B:884:LEU:HD11	1:B:889:LEU:HD23	2.04	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	863/967 (89%)	771 (89%)	76 (9%)	16 (2%)	9	28
1	B	842/967 (87%)	701 (83%)	107 (13%)	34 (4%)	3	10
All	All	1705/1934 (88%)	1472 (86%)	183 (11%)	50 (3%)	5	16

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	583	ARG
1	A	616	GLU
1	A	617	LYS
1	A	922	GLU
1	A	923	ALA
1	B	535	LYS

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Mol	Chain	Res	Type
1	B	545	LYS
1	B	546	GLY
1	B	569	GLY
1	B	596	SER
1	B	926	SER
1	B	948	ASN
1	A	534	VAL
1	A	619	SER
1	B	100	LEU
1	B	216	PHE
1	B	606	LYS
1	B	616	GLU
1	B	649	GLN
1	B	739	TRP
1	B	776	GLN
1	B	860	HIS
1	A	603	HIS
1	A	605	LEU
1	B	72	VAL
1	B	155	LYS
1	B	239	VAL
1	B	245	GLU
1	B	278	THR
1	B	694	PRO
1	A	55	VAL
1	A	155	LYS
1	B	60	GLU
1	B	921	LEU
1	B	945	LEU
1	B	470	GLY
1	B	598	ASN
1	B	720	GLU
1	B	730	PHE
1	B	732	PRO
1	A	60	GLU
1	B	99	VAL
1	B	615	PRO
1	B	692	SER
1	A	715	ILE
1	B	715	ILE
1	A	175	GLY
1	B	898	ILE

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Mol	Chain	Res	Type
1	A	133	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	772/870 (89%)	699 (90%)	73 (10%)	10	26
1	B	733/870 (84%)	675 (92%)	58 (8%)	14	36
All	All	1505/1740 (86%)	1374 (91%)	131 (9%)	12	31

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	PHE
1	A	65	GLN
1	A	67	LEU
1	A	73	VAL
1	A	80	LEU
1	A	92	VAL
1	A	110	LEU
1	A	130	TYR
1	A	145	HIS
1	A	194	LEU
1	A	196	VAL
1	A	229	ARG
1	A	243	GLU
1	A	248	LEU
1	A	261	THR
1	A	278	THR
1	A	320	LEU
1	A	322	LYS
1	A	355	THR
1	A	364	VAL
1	A	367	VAL
1	A	383	MET

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Mol	Chain	Res	Type
1	A	395	PHE
1	A	401	LEU
1	A	426	THR
1	A	437	SER
1	A	442	THR
1	A	452	GLU
1	A	479	ILE
1	A	491	LYS
1	A	493	ASP
1	A	528	LEU
1	A	530	GLU
1	A	533	GLU
1	A	552	VAL
1	A	559	LEU
1	A	563	GLN
1	A	582	GLU
1	A	585	LEU
1	A	588	ILE
1	A	591	THR
1	A	593	SER
1	A	598	ASN
1	A	604	ILE
1	A	613	ASP
1	A	618	THR
1	A	624	ASN
1	A	625	VAL
1	A	645	THR
1	A	676	THR
1	A	681	LEU
1	A	697	LEU
1	A	722	LEU
1	A	729	TYR
1	A	742	LYS
1	A	761	LEU
1	A	762	ASN
1	A	767	ILE
1	A	773	LEU
1	A	801	THR
1	A	802	THR
1	A	825	LEU
1	A	834	GLN
1	A	835	GLU

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Mol	Chain	Res	Type
1	A	855	LEU
1	A	859	LEU
1	A	877	ARG
1	A	896	MET
1	A	909	ASP
1	A	916	LEU
1	A	926	SER
1	A	927	HIS
1	A	952	LEU
1	B	58	ASN
1	B	73	VAL
1	B	76	LEU
1	B	80	LEU
1	B	99	VAL
1	B	106	GLN
1	B	110	LEU
1	B	145	HIS
1	B	155	LYS
1	B	169	GLN
1	B	194	LEU
1	B	196	VAL
1	B	215	LEU
1	B	240	LYS
1	B	245	GLU
1	B	261	THR
1	B	268	VAL
1	B	322	LYS
1	B	352	ASP
1	B	364	VAL
1	B	367	VAL
1	B	383	MET
1	B	395	PHE
1	B	401	LEU
1	B	419	ASN
1	B	433	SER
1	B	434	ARG
1	B	436	ILE
1	B	468	PHE
1	B	533	GLU
1	B	540	THR
1	B	559	LEU
1	B	585	LEU

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Mol	Chain	Res	Type
1	B	588	ILE
1	B	598	ASN
1	B	604	ILE
1	B	610	ASP
1	B	621	VAL
1	B	624	ASN
1	B	625	VAL
1	B	633	VAL
1	B	650	ASN
1	B	674	ARG
1	B	675	LEU
1	B	681	LEU
1	B	686	TYR
1	B	697	LEU
1	B	761	LEU
1	B	767	ILE
1	B	825	LEU
1	B	834	GLN
1	B	855	LEU
1	B	871	LEU
1	B	873	TRP
1	B	888	ASP
1	B	909	ASP
1	B	911	LEU
1	B	952	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	169	GLN
1	A	412	GLN
1	A	554	GLN
1	A	562	GLN
1	A	587	HIS
1	A	598	ASN
1	A	624	ASN
1	A	648	ASN
1	A	651	HIS
1	A	664	HIS
1	A	806	ASN
1	A	834	GLN

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Mol	Chain	Res	Type
1	A	854	ASN
1	A	860	HIS
1	A	869	GLN
1	A	870	GLN
1	A	904	HIS
1	A	927	HIS
1	A	959	ASN
1	B	58	ASN
1	B	159	HIS
1	B	203	GLN
1	B	301	GLN
1	B	412	GLN
1	B	419	ASN
1	B	563	GLN
1	B	598	ASN
1	B	624	ASN
1	B	651	HIS
1	B	689	HIS
1	B	728	GLN
1	B	763	HIS
1	B	811	GLN
1	B	822	ASN
1	B	833	HIS
1	B	860	HIS
1	B	870	GLN
1	B	879	ASN
1	B	912	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z  > 2$
2	NAG	A	1001	1,2	14,14,15	0.56	0	15,19,21	0.89	1 (6%)
2	NAG	A	1002	2	14,14,15	0.47	0	15,19,21	0.95	1 (6%)
2	NAG	A	1003	1,2	14,14,15	0.56	0	15,19,21	0.82	0
2	NAG	A	1004	2	14,14,15	0.51	0	15,19,21	0.84	1 (6%)
2	NAG	A	1005	1	14,14,15	0.49	0	15,19,21	0.96	1 (6%)
2	NAG	A	1006	1	14,14,15	0.76	0	15,19,21	0.89	0
2	NAG	A	1007	1	14,14,15	0.48	0	15,19,21	0.94	1 (6%)
4	P52	A	1009	3	33,38,38	4.01	5 (15%)	35,53,53	2.34	6 (17%)
5	IMD	A	1010	-	3,5,5	0.54	0	4,5,5	0.66	0
5	IMD	A	1011	-	3,5,5	0.54	0	4,5,5	0.50	0
6	MAN	B	1001	2,6	11,11,12	0.57	0	13,15,17	2.16	4 (30%)
6	MAN	B	1002	6	11,11,12	0.54	0	13,15,17	2.07	3 (23%)
2	NAG	B	1003	1,2	14,14,15	0.48	0	15,19,21	2.06	3 (20%)
2	NAG	B	1004	2,6	14,14,15	0.54	0	15,19,21	1.43	1 (6%)
2	NAG	B	1005	1,2	14,14,15	0.52	0	15,19,21	0.69	0
2	NAG	B	1006	2	14,14,15	0.58	0	15,19,21	1.08	1 (6%)
2	NAG	B	1007	1	14,14,15	0.55	0	15,19,21	1.25	1 (6%)
2	NAG	B	1008	1	14,14,15	0.47	0	15,19,21	0.80	1 (6%)
4	P52	B	1010	3	33,38,38	4.01	5 (15%)	35,53,53	3.01	5 (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
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	P52	A	1009	3	-	0/29/36/36	0/3/3/3
5	IMD	A	1010	-	-	0/0/0/0	0/1/1/1
5	IMD	A	1011	-	-	0/0/0/0	0/1/1/1
6	MAN	B	1001	2,6	-	0/2/19/22	0/1/1/1
6	MAN	B	1002	6	-	0/2/19/22	0/1/1/1
2	NAG	B	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	2,6	-	0/6/23/26	0/1/1/1
2	NAG	B	1005	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1006	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
4	P52	B	1010	3	-	0/29/36/36	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1009	P52	P1-C11	-20.69	1.60	1.79
4	B	1010	P52	P1-C11	-20.61	1.60	1.79
4	B	1010	P52	C9-N1	-6.37	1.29	1.47
4	A	1009	P52	C9-N1	-6.32	1.29	1.47
4	B	1010	P52	P1-O1	-2.02	1.46	1.49
4	A	1009	P52	P1-O1	-2.01	1.46	1.49
4	B	1010	P52	C10-N2	3.91	1.42	1.34
4	A	1009	P52	C10-N2	4.20	1.43	1.34
4	A	1009	P52	C18-N4	5.48	1.43	1.32
4	B	1010	P52	C18-N4	5.80	1.44	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	NAG	C4-C3-C2	-4.00	105.16	111.02
4	B	1010	P52	O4-C18-N4	-2.99	118.49	123.06
4	A	1009	P52	O4-C18-N4	-2.73	118.88	123.06
6	B	1002	MAN	C6-C5-C4	-2.64	106.82	113.00
4	A	1009	P52	O3-C10-N2	-2.60	118.02	122.90
6	B	1002	MAN	C2-C3-C4	-2.51	106.50	110.88
4	B	1010	P52	O3-C10-N2	-2.31	118.56	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1009	P 52	C1-C2-C7	-2.03	116.17	121.24
2	A	1002	NAG	C1-O5-C5	2.05	114.98	112.17
2	A	1001	NAG	C1-O5-C5	2.10	115.07	112.17
2	A	1004	NAG	C1-O5-C5	2.13	115.10	112.17
2	B	1008	NAG	C1-O5-C5	2.16	115.15	112.17
6	B	1001	MAN	C3-C4-C5	2.33	114.33	110.22
4	A	1009	P 52	C12-C10-N2	2.50	120.06	116.16
2	A	1007	NAG	C1-O5-C5	2.52	115.64	112.17
4	B	1010	P 52	C12-C10-N2	2.55	120.15	116.16
4	A	1009	P 52	C5-C4-C3	2.57	123.74	120.21
4	B	1010	P 52	C5-C4-C3	2.77	124.02	120.21
2	A	1005	NAG	C1-O5-C5	2.84	116.08	112.17
6	B	1001	MAN	C1-O5-C5	2.91	116.18	112.17
2	B	1003	NAG	C1-C2-N2	2.96	115.54	110.49
2	B	1006	NAG	C1-O5-C5	3.52	117.02	112.17
6	B	1001	MAN	C1-C2-C3	3.61	114.23	109.65
2	B	1007	NAG	O5-C1-C2	3.89	116.89	111.47
6	B	1001	MAN	C2-C3-C4	4.32	118.41	110.88
2	B	1004	NAG	C1-O5-C5	4.56	118.45	112.17
2	B	1003	NAG	C1-O5-C5	5.11	119.21	112.17
6	B	1002	MAN	C1-O5-C5	6.21	120.72	112.17
4	A	1009	P 52	C17-N2-C10	11.61	147.10	121.66
4	B	1010	P 52	C17-N2-C10	16.05	156.83	121.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1009	P 52	3	0
6	B	1001	MAN	3	0
6	B	1002	MAN	2	0
2	B	1003	NAG	1	0
2	B	1005	NAG	3	0
2	B	1006	NAG	1	0
4	B	1010	P 52	2	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<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%)	-0.02	15 (1%) 70 66	21, 48, 86, 115	2 (0%)
1	B	854/967 (88%)	0.76	117 (13%) 3 2	29, 84, 120, 144	0
All	All	1723/1934 (89%)	0.37	132 (7%) 14 9	21, 62, 112, 144	2 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	TRP	12.1
1	B	570	VAL	8.8
1	B	559	LEU	8.4
1	B	687	LEU	7.4
1	B	603	HIS	6.5
1	B	537	MET	6.3
1	B	602	ARG	5.8
1	B	550	LEU	5.5
1	B	534	VAL	5.4
1	B	72	VAL	5.4
1	B	611	THR	5.4
1	B	623	PHE	5.2
1	B	561	LEU	5.2
1	B	635	TYR	5.2
1	B	634	HIS	5.1
1	B	105	THR	5.0
1	B	153	PRO	4.9
1	B	681	LEU	4.8
1	B	622	LYS	4.6
1	B	609	THR	4.5
1	B	610	ASP	4.4
1	B	607	SER	4.3
1	B	73	VAL	4.3
1	B	797	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	637	GLY	4.2
1	B	152	VAL	4.2
1	B	666	VAL	4.2
1	B	613	ASP	4.2
1	B	555	ASP	4.1
1	B	956	LEU	4.0
1	B	924	GLN	4.0
1	B	107	PHE	4.0
1	B	651	HIS	3.9
1	B	767	ILE	3.8
1	B	108	ILE	3.8
1	B	569	GLY	3.8
1	B	831	SER	3.7
1	B	606	LYS	3.6
1	B	944	TRP	3.6
1	B	620	TRP	3.6
1	B	734	ILE	3.6
1	B	952	LEU	3.6
1	B	837	LEU	3.5
1	B	106	GLN	3.5
1	B	532	ALA	3.5
1	A	779	GLU	3.5
1	A	614	LEU	3.4
1	B	500	SER	3.4
1	B	633	VAL	3.4
1	A	556	GLY	3.3
1	A	559	LEU	3.3
1	B	590	LEU	3.2
1	B	416	TYR	3.2
1	B	465	LEU	3.2
1	B	549	LEU	3.2
1	B	677	LEU	3.2
1	B	838	LEU	3.1
1	B	667	PHE	3.1
1	B	768	GLN	3.1
1	A	72	VAL	3.1
1	B	600	ILE	3.0
1	B	648	ASN	3.0
1	B	832	LYS	3.0
1	A	784	LEU	3.0
1	B	380	LEU	3.0
1	B	638	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	120	ALA	3.0
1	B	719	SER	2.9
1	A	618	THR	2.9
1	B	784	LEU	2.9
1	B	162	TYR	2.9
1	B	621	VAL	2.9
1	B	598	ASN	2.9
1	B	689	HIS	2.8
1	B	680	ALA	2.8
1	B	750	LEU	2.8
1	B	541	TRP	2.8
1	B	612	LEU	2.8
1	A	619	SER	2.8
1	B	66	GLU	2.7
1	B	536	GLU	2.7
1	B	670	VAL	2.7
1	B	686	TYR	2.7
1	B	142	TYR	2.7
1	B	724	ARG	2.7
1	B	647	LEU	2.7
1	B	639	GLY	2.7
1	B	945	LEU	2.6
1	B	597	SER	2.6
1	B	156	LEU	2.6
1	B	150	LEU	2.6
1	A	162	TYR	2.5
1	A	612	LEU	2.5
1	B	866	PRO	2.5
1	B	723	LYS	2.5
1	B	721	ASN	2.5
1	B	556	GLY	2.5
1	B	74	ILE	2.5
1	B	101	VAL	2.5
1	B	614	LEU	2.5
1	B	538	MET	2.5
1	B	100	LEU	2.4
1	B	775	SER	2.4
1	B	366	ARG	2.4
1	B	644	ILE	2.4
1	B	641	ASP	2.4
1	B	684	THR	2.4
1	B	588	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	605	LEU	2.4
1	B	954	THR	2.4
1	B	102	SER	2.4
1	A	555	ASP	2.3
1	B	828	LEU	2.3
1	A	647	LEU	2.3
1	B	671	GLY	2.3
1	A	552	VAL	2.3
1	B	865	ARG	2.3
1	B	774	PHE	2.3
1	B	599	VAL	2.3
1	A	617	LYS	2.2
1	B	64	TRP	2.2
1	B	799	ALA	2.2
1	B	696	LEU	2.2
1	B	636	GLU	2.1
1	B	727	LEU	2.1
1	B	739	TRP	2.1
1	B	560	ARG	2.1
1	B	615	PRO	2.1
1	B	441	GLU	2.1
1	B	619	SER	2.0
1	A	108	ILE	2.0
1	B	643	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
4	P52	B	1010	36/36	0.95	0.32	2.43	33,57,88,90	4
4	P52	A	1009	36/36	0.95	0.31	2.24	25,38,60,66	3
5	IMD	A	1010	5/5	0.79	0.24	1.61	64,68,69,80	0
2	NAG	A	1002	14/15	0.88	0.21	1.32	62,80,91,93	0
2	NAG	A	1005	14/15	0.94	0.17	0.26	65,78,82,84	0
2	NAG	A	1001	14/15	0.95	0.19	0.18	39,61,68,68	0
2	NAG	B	1004	14/15	0.90	0.15	0.01	48,71,91,97	0
3	ZN	B	1009	1/1	0.98	0.23	-0.11	47,47,47,47	0
3	ZN	A	1008	1/1	1.00	0.22	-0.12	25,25,25,25	0
5	IMD	A	1011	5/5	0.91	0.22	-0.24	57,60,69,70	0
2	NAG	B	1005	14/15	0.91	0.16	-0.34	67,85,101,103	0
2	NAG	B	1003	14/15	0.94	0.14	-0.43	36,53,63,63	0
2	NAG	A	1003	14/15	0.97	0.15	-0.62	40,47,62,64	0
2	NAG	B	1007	14/15	0.77	0.27	-	85,112,123,137	0
2	NAG	A	1004	14/15	0.94	0.14	-	50,63,70,72	0
6	MAN	B	1002	11/12	0.70	0.33	-	91,109,129,132	0
2	NAG	B	1008	14/15	0.83	0.29	-	79,109,118,122	0
2	NAG	A	1007	14/15	0.85	0.18	-	80,105,111,113	0
6	MAN	B	1001	11/12	0.83	0.17	-	70,86,98,107	0
2	NAG	B	1006	14/15	0.86	0.20	-	62,94,102,102	0
2	NAG	A	1006	14/15	0.88	0.27	-	76,88,106,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.