



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 AM GMT

PDB ID : 3EG9  
Title : Crystal structure of the mammalian COPII-coat protein Sec23/24 bound to the transport signal sequence of membrin  
Authors : Goldberg, J.; Mancias, J.D.  
Deposited on : 2008-09-10  
Resolution : 3.00 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

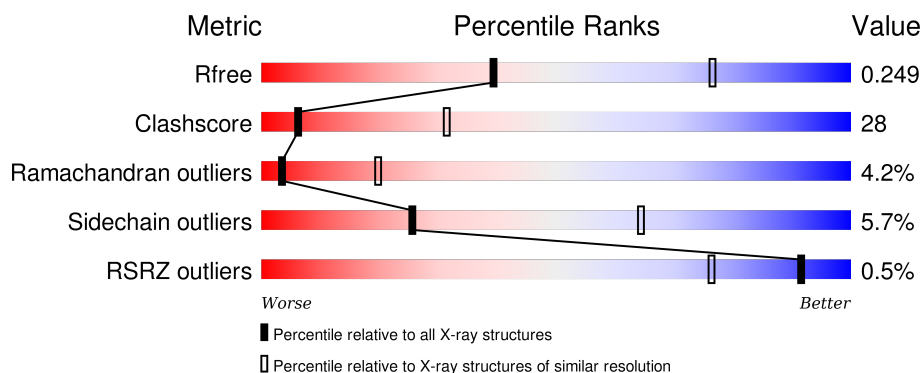
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	764	<div> <div></div> <div>54% 36% 5%</div> </div>
2	B	770	<div> <div></div> <div>52% 41% 7%</div> </div>
3	C	7	<div> <div></div> <div>29% 57% 14%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11956 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5764	3672	992	1060	40			

- Molecule 2 is a protein called SEC24 related gene family, member D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	767	Total	C	N	O	S	0	0	0
			6038	3841	1024	1119	54			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	EXPRESSION TAG	UNP Q8IYI7
B	2	MET	-	EXPRESSION TAG	UNP Q8IYI7
B	3	GLY	-	EXPRESSION TAG	UNP Q8IYI7

- Molecule 3 is a protein called peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	S	0	0	0
			45	28	6	10	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

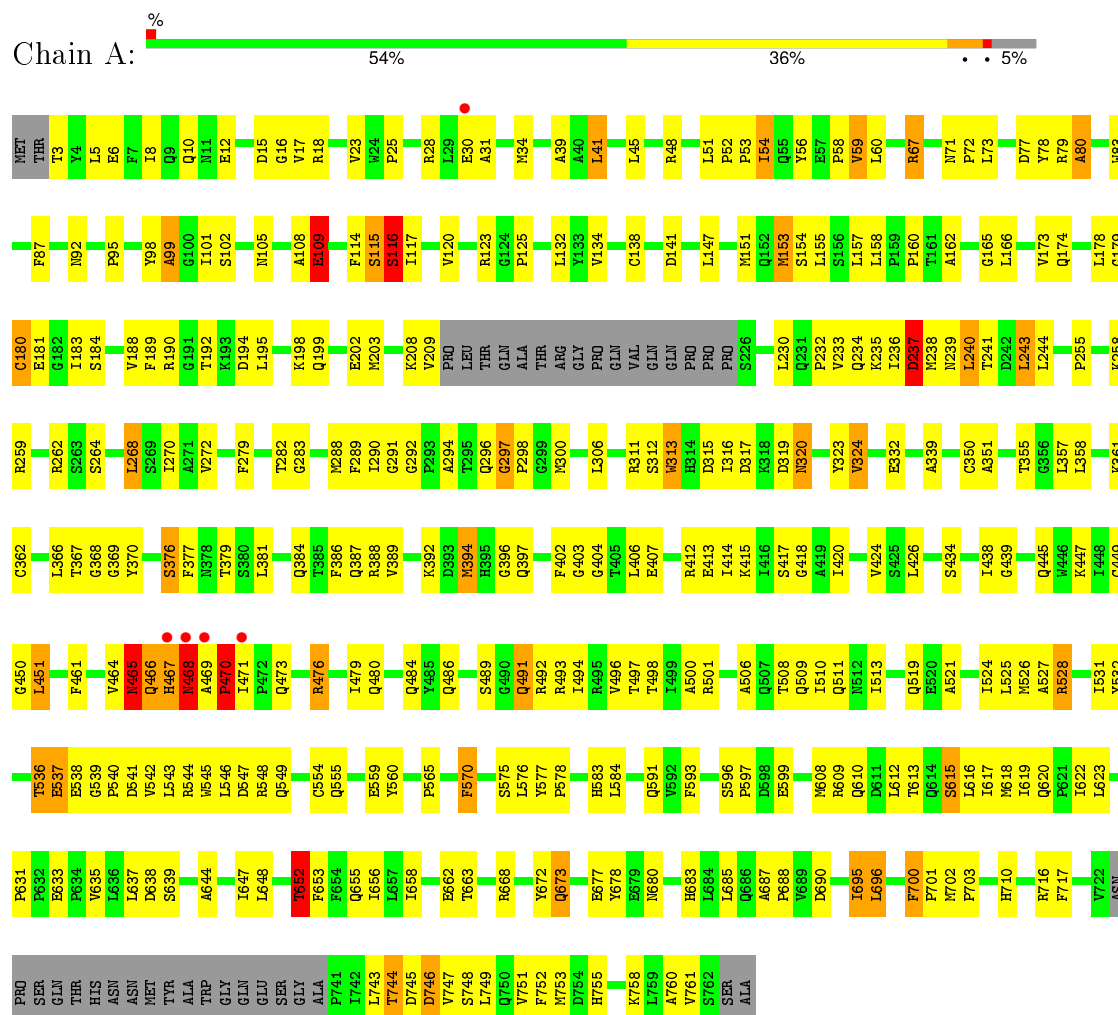
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total 51	O 51	0	0
5	B	55	Total 55	O 55	0	0
5	C	1	Total 1	O 1	0	0

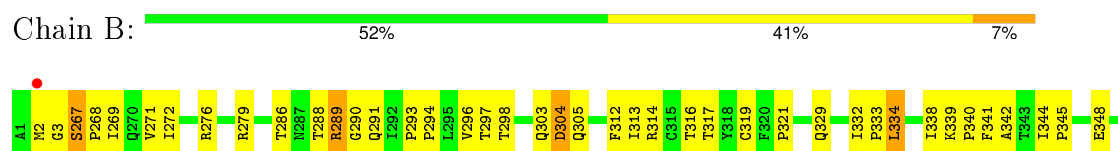
### 3 Residue-property plots

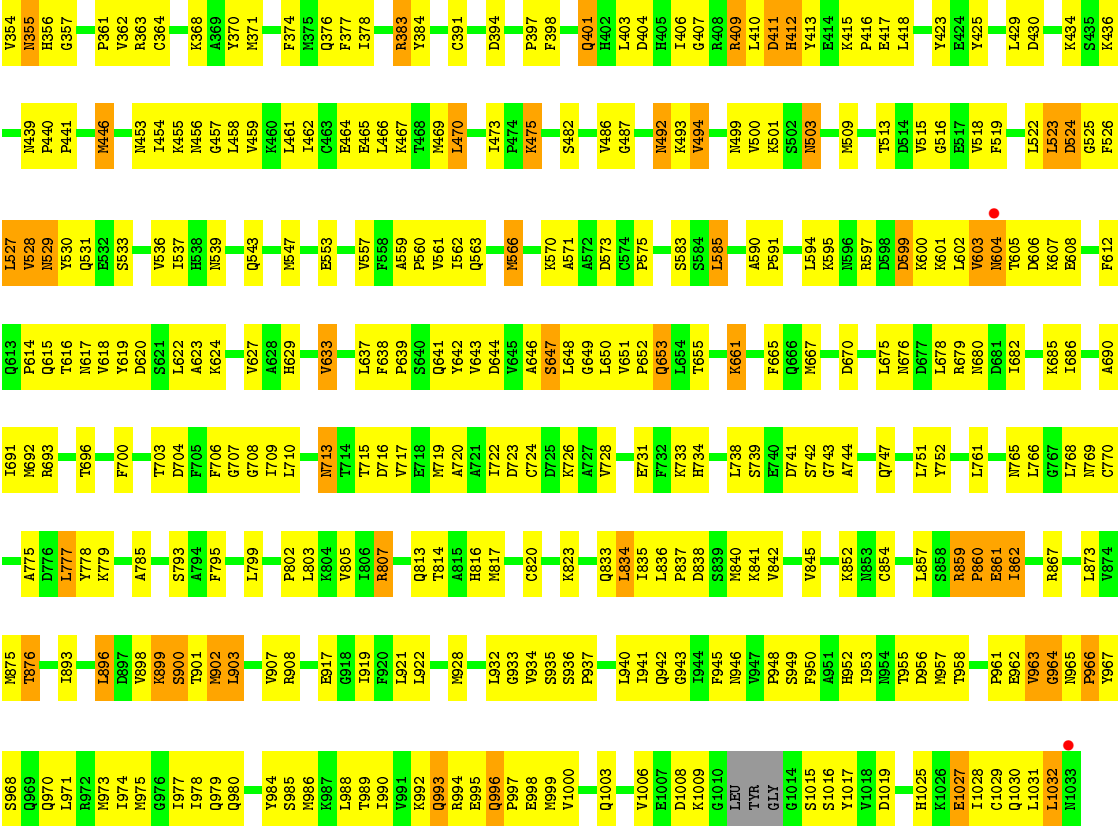
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Protein transport protein Sec23A

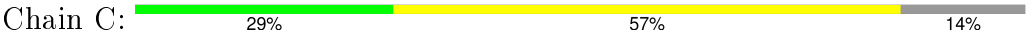


#### • Molecule 2: SEC24 related gene family, member D





• Molecule 3: peptide



T116
T117
I118
P119
M120
D121
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.13Å 140.75Å 152.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 45.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 95.9 (45.58-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.254 0.199 , 0.249	Depositor DCC
$R_{free}$ test set	2161 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45074 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.38	0/5901	0.66	4/7995 (0.1%)
2	B	0.39	0/6166	0.67	0/8351
3	C	0.43	0/45	0.75	0/61
All	All	0.38	0/12112	0.67	4/16407 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-7.66	90.32	111.00
1	A	652	THR	N-CA-C	-5.62	95.84	111.00
1	A	465	ASN	N-CA-C	-5.46	96.27	111.00
1	A	367	THR	N-CA-C	-5.27	96.78	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5764	0	5715	269	0
2	B	6038	0	6038	398	0
3	C	45	0	44	11	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	51	0	0	7	0
5	B	55	0	0	7	0
5	C	1	0	0	1	0
All	All	11956	0	11797	663	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 28.

All (663) 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)
2:B:317:THR:HG22	2:B:319:CYS:H	1.23	1.02
2:B:267:SER:HB2	2:B:908:ARG:HE	1.22	1.01
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.42	0.97
1:A:54:ILE:HG13	1:A:54:ILE:O	1.65	0.95
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.47	0.94
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.51	0.93
2:B:633:VAL:H	2:B:655:THR:HG21	1.35	0.91
2:B:2:MET:HE1	2:B:836:LEU:HD12	1.51	0.90
2:B:713:ASN:HD21	2:B:716:ASP:H	1.12	0.90
1:A:123:ARG:HG3	1:A:125:PRO:HD2	1.53	0.90
1:A:381:LEU:HA	1:A:702:MET:HE2	1.54	0.90
2:B:453:ASN:ND2	2:B:583:SER:HB3	1.89	0.88
2:B:453:ASN:HD21	2:B:583:SER:HB3	1.36	0.88
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.57	0.87
2:B:901:THR:HG22	2:B:902:MET:H	1.36	0.87
2:B:743:GLY:HA2	2:B:770:CYS:HB2	1.57	0.87
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.56	0.86
2:B:802:PRO:HB2	2:B:805:VAL:HG23	1.55	0.85
1:A:283:GLY:H	1:A:486:GLN:HE22	1.20	0.85
1:A:3:THR:HB	1:A:6:GLU:HG3	1.58	0.85
1:A:381:LEU:HA	1:A:702:MET:CE	2.06	0.84
2:B:2:MET:HE2	3:C:118:ILE:HD11	1.58	0.84
2:B:963:VAL:HG12	2:B:964:GLY:H	1.43	0.84
2:B:454:ILE:HD13	2:B:459:VAL:HG21	1.60	0.83
1:A:596:SER:OG	1:A:599:GLU:HG3	1.79	0.82
2:B:462:ILE:O	2:B:466:LEU:HB2	1.81	0.81
2:B:595:LYS:H	2:B:615:GLN:HE22	1.28	0.81
1:A:747:VAL:HG12	1:A:748:SER:H	1.43	0.81
1:A:236:ILE:HG22	1:A:240:LEU:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:VAL:HG11	2:B:537:ILE:HG12	1.62	0.80
2:B:404:ASP:OD2	2:B:410:LEU:HB2	1.83	0.79
2:B:1000:VAL:HA	2:B:1003:GLN:HE21	1.45	0.79
2:B:2:MET:CE	2:B:836:LEU:HD12	2.13	0.78
1:A:115:SER:O	1:A:116:SER:HB2	1.83	0.78
2:B:355:ASN:ND2	2:B:357:GLY:H	1.80	0.78
2:B:713:ASN:ND2	2:B:716:ASP:H	1.81	0.78
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.13	0.77
2:B:267:SER:HB2	2:B:908:ARG:NE	1.99	0.77
2:B:446:MET:HE3	2:B:561:VAL:HG12	1.65	0.77
2:B:523:LEU:O	2:B:524:ASP:HB2	1.84	0.77
2:B:633:VAL:H	2:B:655:THR:CG2	1.99	0.75
1:A:312:SER:O	1:A:316:ILE:HG22	1.87	0.75
2:B:1030:GLN:C	2:B:1032:LEU:H	1.87	0.75
2:B:2:MET:HG2	2:B:1017:TYR:OH	1.86	0.75
1:A:656:ILE:HD11	1:A:695:ILE:HD13	1.68	0.75
2:B:345:PRO:HB2	2:B:348:GLU:HG3	1.68	0.73
1:A:528:ARG:HA	1:A:608:MET:HE1	1.68	0.73
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.69	0.73
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.70	0.73
2:B:356:HIS:HD2	2:B:362:VAL:H	1.36	0.73
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.03	0.72
1:A:238:MET:O	1:A:241:THR:HG22	1.90	0.72
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.72	0.72
2:B:852:LYS:HE3	2:B:1015:SER:O	1.90	0.71
2:B:600:LYS:HG3	2:B:600:LYS:O	1.90	0.71
1:A:30:GLU:CD	1:A:506:ALA:HB3	2.10	0.71
1:A:407:GLU:HG3	1:A:445:GLN:HG3	1.70	0.71
2:B:600:LYS:HA	2:B:859:ARG:NH1	2.05	0.71
2:B:933:GLY:O	2:B:936:SER:HB2	1.89	0.71
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.20	0.71
2:B:600:LYS:HD2	2:B:602:LEU:HD21	1.72	0.71
2:B:312:PHE:CZ	2:B:344:ILE:HD11	2.25	0.71
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.72	0.71
1:A:511:GLN:H	1:A:511:GLN:CD	1.94	0.70
2:B:378:ILE:HG12	2:B:383:ARG:O	1.91	0.70
2:B:943:GLY:O	2:B:968:SER:HB2	1.91	0.70
1:A:583:HIS:HD2	1:A:620:GLN:HE21	1.40	0.70
2:B:686:ILE:HG22	2:B:723:ASP:HB3	1.73	0.70
1:A:283:GLY:N	1:A:486:GLN:HE22	1.89	0.70
1:A:190:ARG:HH12	2:B:519:PHE:HB3	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ASP:CG	1:A:746:ASP:H	1.96	0.69
2:B:599:ASP:HB3	2:B:601:LYS:HG3	1.72	0.69
2:B:269:ILE:HD11	2:B:907:VAL:C	2.12	0.69
1:A:565:PRO:HG3	1:A:758:LYS:HA	1.75	0.69
2:B:837:PRO:HG2	2:B:840:MET:HG3	1.74	0.69
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.29	0.68
1:A:3:THR:HG22	1:A:5:LEU:H	1.58	0.68
1:A:181:GLU:HG2	1:A:239:ASN:HD21	1.58	0.68
2:B:719:MET:SD	2:B:722:ILE:HD12	2.34	0.68
2:B:456:ASN:OD1	2:B:458:LEU:HB2	1.94	0.68
1:A:418:GLY:HA3	1:A:438:ILE:O	1.92	0.68
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.75	0.68
2:B:605:THR:HG22	2:B:607:LYS:HB3	1.75	0.67
2:B:469:MET:HE2	2:B:678:LEU:HG	1.75	0.67
2:B:269:ILE:HD11	2:B:908:ARG:N	2.10	0.67
2:B:616:THR:HB	2:B:618:VAL:HG22	1.77	0.67
1:A:179:GLY:O	1:A:181:GLU:HG3	1.95	0.67
2:B:469:MET:CE	2:B:678:LEU:HG	2.25	0.67
2:B:963:VAL:O	2:B:964:GLY:O	2.13	0.67
2:B:500:VAL:HG11	2:B:537:ILE:CG1	2.25	0.67
1:A:466:GLN:O	1:A:468:ASN:N	2.27	0.67
2:B:842:VAL:HG12	2:B:842:VAL:O	1.95	0.67
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.77	0.67
2:B:601:LYS:HB3	2:B:605:THR:HG21	1.77	0.67
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.77	0.67
1:A:583:HIS:CD2	1:A:620:GLN:HG3	2.30	0.66
2:B:267:SER:CB	2:B:908:ARG:HE	2.05	0.66
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.76	0.66
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.13	0.66
2:B:501:LYS:CD	2:B:503:ASN:HD21	2.09	0.66
1:A:743:LEU:O	1:A:744:THR:HB	1.95	0.66
2:B:963:VAL:HG12	2:B:964:GLY:N	2.09	0.66
2:B:845:VAL:HG22	2:B:1017:TYR:CZ	2.31	0.66
2:B:2:MET:SD	2:B:3:GLY:N	2.69	0.65
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.77	0.65
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.78	0.65
2:B:835:ILE:HD13	3:C:117:THR:HG23	1.77	0.65
2:B:860:PRO:O	2:B:861:GLU:HB2	1.95	0.65
1:A:30:GLU:OE1	1:A:506:ALA:HB3	1.96	0.65
1:A:369:GLY:O	1:A:609:ARG:NH2	2.29	0.65
2:B:775:ALA:O	2:B:779:LYS:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:LEU:HD12	2:B:974:ILE:HD11	1.79	0.65
1:A:652:THR:HG23	1:A:655:GLN:H	1.61	0.65
2:B:992:LYS:HD2	2:B:996:GLN:NE2	2.11	0.65
2:B:446:MET:CE	2:B:561:VAL:HG12	2.27	0.65
1:A:700:PHE:O	1:A:702:MET:N	2.30	0.64
2:B:802:PRO:HD2	2:B:805:VAL:HG21	1.78	0.64
1:A:190:ARG:NH1	2:B:519:PHE:HB3	2.13	0.64
2:B:974:ILE:HA	2:B:977:ILE:HG22	1.78	0.64
2:B:334:LEU:HD22	2:B:334:LEU:H	1.62	0.64
2:B:2:MET:CE	3:C:118:ILE:HD11	2.27	0.64
2:B:901:THR:HG22	2:B:902:MET:N	2.09	0.64
2:B:605:THR:C	2:B:607:LYS:H	1.97	0.64
1:A:468:ASN:C	1:A:470:PRO:HD3	2.18	0.64
2:B:901:THR:HG22	2:B:903:LEU:H	1.62	0.64
1:A:656:ILE:HG13	1:A:695:ILE:HG21	1.79	0.63
2:B:945:PHE:HE2	2:B:990:ILE:HD13	1.63	0.63
3:C:116:THR:N	5:C:4:HOH:O	2.31	0.63
1:A:492:ARG:HD3	5:A:811:HOH:O	1.98	0.63
2:B:633:VAL:HG13	2:B:655:THR:HG21	1.80	0.63
1:A:297:GLY:CA	1:A:300:MET:HB2	2.29	0.63
2:B:893:ILE:O	2:B:896:LEU:HB2	1.97	0.63
2:B:602:LEU:N	2:B:605:THR:OG1	2.32	0.63
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.80	0.62
2:B:469:MET:HE3	2:B:679:ARG:HA	1.81	0.62
2:B:321:PRO:HG2	2:B:734:HIS:HE1	1.63	0.62
1:A:190:ARG:HB3	1:A:192:THR:HG22	1.80	0.62
2:B:633:VAL:CG1	2:B:655:THR:HG21	2.29	0.62
2:B:601:LYS:O	2:B:608:GLU:HA	2.00	0.62
2:B:602:LEU:HD23	2:B:602:LEU:N	2.13	0.62
2:B:902:MET:HG2	2:B:902:MET:O	1.99	0.62
2:B:713:ASN:C	2:B:713:ASN:HD22	2.03	0.61
1:A:199:GLN:HB3	1:A:203:MET:HE2	1.82	0.61
2:B:374:PHE:CE2	2:B:765:ASN:HB3	2.35	0.61
2:B:641:GLN:HG2	2:B:642:TYR:N	2.16	0.61
1:A:746:ASP:HB3	5:A:840:HOH:O	1.99	0.61
2:B:453:ASN:O	2:B:459:VAL:HG23	2.01	0.61
1:A:609:ARG:HG3	1:A:609:ARG:HH11	1.66	0.60
1:A:25:PRO:CG	1:A:31:ALA:HB2	2.30	0.60
2:B:355:ASN:C	2:B:355:ASN:HD22	2.04	0.60
1:A:297:GLY:N	1:A:300:MET:HB2	2.16	0.60
1:A:116:SER:N	5:A:805:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:LEU:HD11	2:B:859:ARG:HB2	1.84	0.60
2:B:492:ASN:O	2:B:493:LYS:HG2	2.01	0.60
1:A:160:PRO:HB3	1:A:234:GLN:HB3	1.83	0.60
1:A:638:ASP:OD1	1:A:639:SER:N	2.35	0.60
1:A:155:LEU:HD12	1:A:158:LEU:HD12	1.83	0.60
2:B:600:LYS:HD2	2:B:602:LEU:CD2	2.31	0.60
2:B:835:ILE:O	2:B:836:LEU:HD23	2.01	0.60
1:A:123:ARG:HG2	5:A:811:HOH:O	2.01	0.60
1:A:412:ARG:HG3	1:A:413:GLU:OE2	2.02	0.60
1:A:116:SER:HA	1:A:496:VAL:O	2.02	0.59
2:B:470:LEU:HD12	2:B:473:ILE:HD11	1.84	0.59
2:B:403:LEU:HB3	2:B:407:GLY:HA2	1.84	0.59
2:B:992:LYS:HD2	2:B:996:GLN:HE21	1.67	0.59
2:B:997:PRO:O	2:B:999:MET:N	2.35	0.59
1:A:559:GLU:O	1:A:560:TYR:HB3	2.02	0.59
2:B:690:ALA:HB2	2:B:752:TYR:HB3	1.83	0.59
1:A:283:GLY:H	1:A:486:GLN:NE2	1.97	0.59
1:A:745:ASP:O	1:A:747:VAL:HG23	2.02	0.59
2:B:693:ARG:HG3	2:B:693:ARG:HH11	1.68	0.59
1:A:291:GLY:O	1:A:351:ALA:HB2	2.03	0.59
1:A:617:ILE:HG12	1:A:622:ILE:HD11	1.84	0.59
2:B:901:THR:HB	2:B:970:GLN:HE21	1.68	0.59
1:A:72:PRO:HD3	1:A:109:GLU:O	2.02	0.59
2:B:434:LYS:O	2:B:436:LYS:HG3	2.03	0.58
1:A:54:ILE:HD12	1:A:56:TYR:CZ	2.38	0.58
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.84	0.58
1:A:58:PRO:O	1:A:59:VAL:HB	2.02	0.58
2:B:406:ILE:HG22	2:B:406:ILE:O	2.03	0.58
1:A:536:THR:HG22	1:A:537:GLU:N	2.17	0.58
2:B:964:GLY:HA3	2:B:968:SER:HB3	1.86	0.58
1:A:312:SER:H	1:A:315:ASP:HB2	1.69	0.58
2:B:641:GLN:HG2	2:B:642:TYR:H	1.69	0.58
2:B:356:HIS:CD2	2:B:361:PRO:HA	2.38	0.58
2:B:501:LYS:HD3	2:B:503:ASN:HD21	1.68	0.58
2:B:974:ILE:HA	2:B:977:ILE:CG2	2.33	0.58
1:A:183:ILE:HD11	2:B:509:MET:HB2	1.86	0.58
2:B:854:CYS:O	2:B:867:ARG:HD2	2.04	0.58
2:B:713:ASN:ND2	2:B:715:THR:H	2.02	0.58
1:A:560:TYR:CD1	1:A:761:VAL:HG12	2.39	0.58
2:B:492:ASN:O	2:B:492:ASN:OD1	2.22	0.58
1:A:700:PHE:O	1:A:701:PRO:C	2.40	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:898:VAL:HG22	2:B:967:TYR:CE2	2.39	0.58
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.38	0.57
2:B:962:GLU:HG2	2:B:963:VAL:N	2.18	0.57
1:A:297:GLY:H	1:A:300:MET:HB2	1.68	0.57
2:B:494:VAL:HG22	2:B:513:THR:HA	1.86	0.57
2:B:835:ILE:CD1	3:C:117:THR:HG23	2.34	0.57
1:A:696:LEU:HD12	1:A:703:PRO:HG2	1.87	0.57
2:B:1027:GLU:O	2:B:1031:LEU:HG	2.05	0.57
2:B:371:MET:HB3	2:B:425:TYR:OH	2.04	0.57
1:A:539:GLY:O	1:A:542:VAL:HG23	2.04	0.57
2:B:345:PRO:HD2	2:B:348:GLU:OE1	2.05	0.57
2:B:641:GLN:O	2:B:643:VAL:HG23	2.04	0.57
1:A:744:THR:HG21	1:A:752:PHE:HD1	1.70	0.57
2:B:854:CYS:HB3	2:B:862:ILE:HD13	1.87	0.57
1:A:162:ALA:O	1:A:233:VAL:HG23	2.05	0.56
2:B:410:LEU:HG	2:B:410:LEU:O	2.05	0.56
1:A:466:GLN:HA	1:A:466:GLN:OE1	2.04	0.56
2:B:493:LYS:HA	2:B:557:VAL:HG13	1.87	0.56
2:B:993:GLN:HG2	2:B:994:ARG:N	2.20	0.56
2:B:356:HIS:HE1	2:B:417:GLU:OE2	1.88	0.56
2:B:1030:GLN:C	2:B:1032:LEU:N	2.58	0.56
2:B:934:VAL:HG23	2:B:935:SER:N	2.19	0.56
2:B:333:PRO:HD3	2:B:813:GLN:NE2	2.21	0.56
2:B:965:ASN:HB3	2:B:966:PRO:HD3	1.86	0.56
2:B:775:ALA:HB1	2:B:779:LYS:HE3	1.87	0.56
2:B:922:LEU:C	2:B:922:LEU:HD23	2.26	0.56
2:B:616:THR:HG22	2:B:617:ASN:N	2.21	0.56
1:A:545:TRP:O	1:A:549:GLN:HG2	2.06	0.56
2:B:639:PRO:CB	2:B:643:VAL:HG21	2.28	0.56
2:B:766:LEU:CD2	2:B:768:LEU:HD21	2.36	0.55
1:A:506:ALA:O	1:A:510:ILE:HG13	2.06	0.55
1:A:77:ASP:OD2	1:A:80:ALA:HB3	2.06	0.55
2:B:948:PRO:HG2	2:B:952:HIS:ND1	2.21	0.55
2:B:838:ASP:HA	2:B:841:LYS:HG3	1.87	0.55
2:B:652:PRO:HA	2:B:655:THR:HG22	1.88	0.55
2:B:605:THR:HG22	2:B:607:LYS:CB	2.36	0.55
2:B:928:MET:O	2:B:988:LEU:HD12	2.06	0.55
1:A:8:ILE:HG21	1:A:18:ARG:NH2	2.21	0.55
2:B:963:VAL:CG1	2:B:964:GLY:H	2.15	0.55
2:B:948:PRO:HG2	2:B:952:HIS:CE1	2.42	0.55
2:B:852:LYS:HE2	2:B:1008:ASP:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:MET:HE1	2:B:679:ARG:N	2.21	0.55
1:A:404:GLY:HA2	1:A:484:GLN:O	2.07	0.55
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.72	0.55
1:A:30:GLU:HB3	5:A:835:HOH:O	2.06	0.55
1:A:510:ILE:HB	1:A:511:GLN:NE2	2.22	0.55
2:B:616:THR:HG21	5:B:1107:HOH:O	2.06	0.55
1:A:673:GLN:HG2	1:A:685:LEU:CD1	2.36	0.55
2:B:854:CYS:CB	2:B:862:ILE:HD13	2.36	0.55
1:A:153:MET:HE1	1:A:154:SER:HA	1.89	0.55
1:A:115:SER:O	1:A:116:SER:CB	2.52	0.55
2:B:269:ILE:CD1	2:B:908:ARG:N	2.70	0.54
2:B:992:LYS:HB2	2:B:996:GLN:HE21	1.72	0.54
2:B:458:LEU:HD21	2:B:638:PHE:CD2	2.43	0.54
2:B:859:ARG:HB3	2:B:860:PRO:HD3	1.90	0.54
2:B:616:THR:HG22	2:B:617:ASN:H	1.73	0.54
2:B:971:LEU:O	2:B:974:ILE:HG12	2.07	0.54
2:B:340:PRO:HB2	2:B:341:PHE:HD1	1.72	0.54
2:B:453:ASN:CG	2:B:583:SER:HB3	2.28	0.54
2:B:469:MET:HE2	2:B:682:ILE:HD12	1.89	0.54
1:A:350:CYS:HB2	1:A:377:PHE:CE1	2.42	0.54
1:A:536:THR:O	1:A:538:GLU:N	2.41	0.54
1:A:491:GLN:HG2	1:A:493:ARG:HE	1.73	0.54
2:B:606:ASP:HA	2:B:802:PRO:HG3	1.90	0.54
1:A:745:ASP:CG	1:A:746:ASP:N	2.61	0.54
2:B:526:PHE:O	2:B:527:LEU:HB2	2.09	0.54
1:A:53:PRO:O	1:A:54:ILE:C	2.47	0.53
2:B:685:LYS:HG3	5:B:1116:HOH:O	2.07	0.53
2:B:355:ASN:HD22	2:B:356:HIS:N	2.06	0.53
2:B:974:ILE:O	2:B:978:ILE:HG13	2.07	0.53
2:B:901:THR:CG2	2:B:902:MET:H	2.14	0.53
1:A:296:GLN:HA	1:A:300:MET:HE2	1.90	0.53
2:B:898:VAL:O	2:B:899:LYS:C	2.46	0.53
2:B:529:ASN:HD21	2:B:531:GLN:HG2	1.73	0.53
2:B:312:PHE:HZ	2:B:344:ILE:HD11	1.71	0.53
2:B:955:THR:C	2:B:957:MET:H	2.12	0.53
2:B:465:GLU:HG2	2:B:675:LEU:HD22	1.90	0.53
2:B:962:GLU:HG2	2:B:963:VAL:H	1.74	0.53
2:B:334:LEU:HD22	2:B:334:LEU:N	2.24	0.53
2:B:958:THR:HG21	2:B:988:LEU:O	2.09	0.53
2:B:1000:VAL:HA	2:B:1003:GLN:NE2	2.21	0.53
2:B:267:SER:CB	2:B:908:ARG:HH21	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HG	1:A:151:MET:CE	2.39	0.53
1:A:386:PHE:O	1:A:389:VAL:HB	2.09	0.53
1:A:524:ILE:HD13	1:A:619:ILE:HD12	1.90	0.53
2:B:623:ALA:O	2:B:627:VAL:HG23	2.09	0.53
2:B:317:THR:HG22	2:B:319:CYS:N	2.08	0.52
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.91	0.52
2:B:955:THR:O	2:B:957:MET:N	2.42	0.52
2:B:814:THR:HA	2:B:817:MET:HE3	1.91	0.52
2:B:917:GLU:HA	2:B:935:SER:O	2.08	0.52
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.38	0.52
1:A:28:ARG:HB3	1:A:466:GLN:OE1	2.09	0.52
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.92	0.52
2:B:340:PRO:HB2	2:B:341:PHE:CD1	2.44	0.52
2:B:996:GLN:CB	2:B:997:PRO:HD2	2.31	0.52
1:A:745:ASP:O	1:A:747:VAL:N	2.43	0.52
1:A:236:ILE:CG2	1:A:240:LEU:HB2	2.38	0.52
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.44	0.52
1:A:239:ASN:HB3	5:A:822:HOH:O	2.08	0.52
1:A:536:THR:HG22	1:A:537:GLU:H	1.75	0.52
2:B:743:GLY:HA2	2:B:770:CYS:CB	2.37	0.52
1:A:521:ALA:HA	1:A:612:LEU:HD12	1.92	0.52
1:A:612:LEU:HD23	1:A:612:LEU:C	2.30	0.52
2:B:703:THR:HG21	2:B:733:LYS:HB2	1.92	0.52
2:B:643:VAL:O	2:B:643:VAL:HG12	2.09	0.52
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.43	0.52
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.91	0.52
2:B:332:ILE:HD11	2:B:778:TYR:CE1	2.45	0.52
2:B:608:GLU:OE1	2:B:803:LEU:HG	2.10	0.52
1:A:60:LEU:HB2	1:A:67:ARG:NH1	2.25	0.52
2:B:339:LYS:HD3	2:B:724:CYS:O	2.10	0.52
2:B:529:ASN:ND2	2:B:531:GLN:H	2.08	0.51
1:A:53:PRO:O	1:A:54:ILE:O	2.27	0.51
2:B:2:MET:HB2	3:C:118:ILE:HD11	1.91	0.51
2:B:605:THR:C	2:B:607:LYS:N	2.63	0.51
1:A:297:GLY:H	1:A:300:MET:CE	2.22	0.51
2:B:693:ARG:HG3	2:B:693:ARG:NH1	2.26	0.51
2:B:633:VAL:HG11	2:B:651:VAL:HG12	1.92	0.51
2:B:600:LYS:O	2:B:600:LYS:CG	2.58	0.51
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.92	0.51
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.10	0.51
1:A:51:LEU:HD21	1:A:117:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:VAL:N	2:B:655:THR:HG21	2.16	0.51
2:B:458:LEU:HD21	2:B:638:PHE:CG	2.45	0.51
1:A:15:ASP:HB3	1:A:497:THR:HG21	1.93	0.51
2:B:430:ASP:N	2:B:430:ASP:OD2	2.44	0.51
2:B:570:LYS:HE2	2:B:629:HIS:CE1	2.45	0.51
2:B:1009:LYS:HE2	2:B:1019:ASP:OD2	2.10	0.51
1:A:536:THR:C	1:A:538:GLU:H	2.14	0.51
1:A:183:ILE:HD12	2:B:547:MET:CE	2.40	0.51
2:B:713:ASN:HD21	2:B:716:ASP:N	1.94	0.51
1:A:25:PRO:HG2	1:A:31:ALA:HB2	1.93	0.51
1:A:368:GLY:HA3	1:A:450:GLY:O	2.11	0.51
2:B:651:VAL:O	2:B:655:THR:HB	2.10	0.51
2:B:1015:SER:HB2	2:B:1019:ASP:HB2	1.92	0.51
2:B:605:THR:CG2	2:B:607:LYS:HB3	2.41	0.51
1:A:755:HIS:CD2	1:A:758:LYS:HE2	2.45	0.51
2:B:751:LEU:HD13	2:B:761:LEU:HD21	1.93	0.51
2:B:807:ARG:HG2	2:B:807:ARG:HH11	1.76	0.51
2:B:339:LYS:HD2	2:B:342:ALA:HB2	1.93	0.51
1:A:524:ILE:CD1	1:A:615:SER:HB3	2.41	0.50
2:B:992:LYS:CB	2:B:996:GLN:HE21	2.23	0.50
1:A:541:ASP:O	1:A:544:ARG:HB3	2.12	0.50
2:B:456:ASN:HB3	5:B:1135:HOH:O	2.10	0.50
2:B:919:ILE:HG12	2:B:932:LEU:HD23	1.93	0.50
1:A:370:TYR:HA	5:A:824:HOH:O	2.10	0.50
2:B:766:LEU:HD21	2:B:768:LEU:HD21	1.93	0.50
2:B:523:LEU:HA	5:B:1109:HOH:O	2.10	0.50
2:B:370:TYR:HB3	2:B:425:TYR:HE1	1.76	0.50
2:B:992:LYS:CD	2:B:996:GLN:HE21	2.23	0.50
1:A:71:ASN:OD1	1:A:73:LEU:HB2	2.11	0.50
1:A:662:GLU:HG3	1:A:710:HIS:CD2	2.47	0.50
2:B:304:ASP:O	2:B:305:GLN:CB	2.58	0.50
1:A:656:ILE:CD1	1:A:695:ILE:HG21	2.42	0.50
2:B:665:PHE:CE1	2:B:670:ASP:HB2	2.46	0.50
2:B:356:HIS:CD2	2:B:362:VAL:H	2.24	0.50
2:B:286:THR:OG1	2:B:304:ASP:O	2.25	0.50
2:B:692:MET:HE1	2:B:728:VAL:HG11	1.93	0.50
1:A:384:GLN:O	1:A:388:ARG:HG3	2.12	0.50
1:A:747:VAL:HG11	1:A:751:VAL:HG11	1.93	0.50
2:B:934:VAL:HG23	2:B:935:SER:H	1.77	0.50
2:B:338:ILE:O	2:B:340:PRO:HD3	2.12	0.50
2:B:529:ASN:HD22	2:B:530:TYR:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ARG:NH2	2:B:368:LYS:HB3	2.27	0.50
2:B:942:GLN:HG2	2:B:948:PRO:HA	1.94	0.49
2:B:543:GLN:HB3	2:B:547:MET:CE	2.42	0.49
2:B:570:LYS:HE2	2:B:629:HIS:NE2	2.27	0.49
1:A:120:VAL:HG11	1:A:491:GLN:OE1	2.12	0.49
1:A:339:ALA:HB1	1:A:424:VAL:HG21	1.95	0.49
2:B:949:SER:O	2:B:952:HIS:HB2	2.13	0.49
2:B:526:PHE:O	2:B:527:LEU:CB	2.61	0.49
1:A:134:VAL:HG11	1:A:288:MET:CE	2.42	0.49
2:B:833:GLN:CD	3:C:117:THR:HG21	2.33	0.49
1:A:656:ILE:CD1	1:A:695:ILE:HD13	2.40	0.49
2:B:661:LYS:HB3	2:B:661:LYS:NZ	2.26	0.49
1:A:3:THR:HG22	1:A:5:LEU:N	2.27	0.49
2:B:500:VAL:HG12	2:B:500:VAL:O	2.11	0.49
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.94	0.49
1:A:476:ARG:HB3	1:A:501:ARG:O	2.13	0.49
3:C:118:ILE:HG22	3:C:120:MET:CE	2.43	0.49
1:A:511:GLN:H	1:A:511:GLN:NE2	2.11	0.49
2:B:627:VAL:HG21	2:B:710:LEU:CD2	2.43	0.49
2:B:276:ARG:HA	2:B:298:THR:HG23	1.95	0.48
1:A:471:ILE:CG2	1:A:473:GLN:HB3	2.43	0.48
2:B:454:ILE:CD1	2:B:459:VAL:HG21	2.38	0.48
2:B:403:LEU:HA	2:B:409:ARG:HA	1.95	0.48
1:A:618:MET:HE3	1:A:653:PHE:CD2	2.48	0.48
2:B:751:LEU:HA	2:B:761:LEU:HD23	1.95	0.48
1:A:232:PRO:HB2	1:A:235:LYS:HB3	1.95	0.48
2:B:842:VAL:CG1	2:B:842:VAL:O	2.61	0.48
1:A:656:ILE:HG13	1:A:695:ILE:CG2	2.42	0.48
1:A:680:ASN:O	1:A:683:HIS:HB2	2.13	0.48
2:B:585:LEU:HD11	2:B:595:LYS:O	2.13	0.48
2:B:355:ASN:C	2:B:355:ASN:ND2	2.67	0.48
2:B:941:ILE:HD13	2:B:950:PHE:HA	1.96	0.48
1:A:417:SER:HB3	1:A:438:ILE:HG13	1.96	0.48
2:B:899:LYS:O	2:B:900:SER:HB3	2.13	0.48
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.95	0.48
2:B:296:VAL:HG12	2:B:314:ARG:NE	2.29	0.48
2:B:383:ARG:HD3	2:B:394:ASP:OD1	2.14	0.48
2:B:751:LEU:HD13	2:B:761:LEU:CD2	2.44	0.48
2:B:499:ASN:HB2	2:B:522:LEU:HD11	1.96	0.48
1:A:198:LYS:HE2	1:A:202:GLU:OE2	2.14	0.48
1:A:41:LEU:HD13	1:A:525:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:PRO:O	2:B:563:GLN:HB3	2.14	0.48
1:A:297:GLY:HA2	1:A:298:PRO:C	2.34	0.47
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.95	0.47
1:A:25:PRO:HG3	1:A:31:ALA:HB2	1.96	0.47
2:B:566:MET:HE1	2:B:570:LYS:HE3	1.96	0.47
1:A:749:LEU:O	1:A:753:MET:HG2	2.14	0.47
1:A:290:ILE:HD12	1:A:355:THR:HB	1.95	0.47
2:B:996:GLN:CB	2:B:997:PRO:CD	2.90	0.47
2:B:651:VAL:N	2:B:652:PRO:HD2	2.29	0.47
1:A:208:LYS:O	1:A:209:VAL:HB	2.14	0.47
1:A:357:LEU:O	1:A:361:LYS:N	2.45	0.47
2:B:288:THR:HG22	2:B:289:ARG:N	2.29	0.47
2:B:834:LEU:HD21	2:B:836:LEU:HD21	1.96	0.47
1:A:236:ILE:O	1:A:237:ASP:C	2.53	0.47
2:B:686:ILE:HD13	5:B:1113:HOH:O	2.14	0.47
2:B:355:ASN:HD22	2:B:357:GLY:H	1.61	0.47
1:A:547:ASP:HB3	1:A:743:LEU:HB2	1.97	0.47
2:B:873:LEU:HD22	2:B:984:TYR:CZ	2.50	0.47
2:B:813:GLN:O	2:B:817:MET:HG3	2.14	0.47
2:B:279:ARG:NH2	2:B:293:PRO:C	2.68	0.47
1:A:509:GLN:O	1:A:510:ILE:C	2.54	0.47
1:A:716:ARG:NE	1:A:717:PHE:CE1	2.83	0.47
2:B:901:THR:CB	2:B:970:GLN:HE21	2.27	0.47
1:A:548:ARG:HH21	1:A:549:GLN:NE2	2.12	0.47
1:A:716:ARG:CZ	1:A:717:PHE:HE1	2.28	0.47
1:A:41:LEU:HD23	1:A:612:LEU:HB2	1.96	0.46
2:B:661:LYS:HB3	2:B:661:LYS:HZ2	1.79	0.46
2:B:516:GLY:HA2	2:B:591:PRO:CD	2.45	0.46
2:B:2:MET:HB2	3:C:118:ILE:CD1	2.45	0.46
2:B:970:GLN:NE2	2:B:973:MET:SD	2.88	0.46
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.50	0.46
2:B:795:PHE:HB3	2:B:875:MET:HE2	1.97	0.46
1:A:548:ARG:HH21	1:A:549:GLN:HE22	1.63	0.46
1:A:527:ALA:O	1:A:531:ILE:HG13	2.15	0.46
2:B:492:ASN:C	2:B:494:VAL:H	2.19	0.46
2:B:494:VAL:CG2	2:B:513:THR:HG22	2.46	0.46
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.98	0.46
2:B:319:CYS:HA	2:B:769:ASN:O	2.15	0.46
2:B:559:ALA:N	2:B:560:PRO:CD	2.78	0.46
2:B:1015:SER:HB2	2:B:1019:ASP:CB	2.45	0.46
2:B:739:SER:C	2:B:741:ASP:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.31	0.46
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.51	0.46
2:B:289:ARG:C	2:B:291:GLN:H	2.19	0.46
2:B:585:LEU:CD2	2:B:594:LEU:HB2	2.46	0.46
1:A:656:ILE:CG1	1:A:695:ILE:HG21	2.43	0.46
2:B:475:LYS:HB3	2:B:482:SER:HB2	1.97	0.46
2:B:934:VAL:C	2:B:936:SER:H	2.19	0.45
2:B:639:PRO:HB3	2:B:643:VAL:CG2	2.30	0.45
2:B:303:GLN:O	2:B:304:ASP:O	2.34	0.45
2:B:515:VAL:CG1	2:B:590:ALA:HB1	2.46	0.45
2:B:415:LYS:HB2	2:B:418:LEU:HD12	1.98	0.45
2:B:528:VAL:HG11	2:B:533:SER:OG	2.15	0.45
1:A:279:PHE:O	1:A:282:THR:HG22	2.16	0.45
1:A:397:GLN:NE2	1:A:489:SER:HB3	2.31	0.45
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.97	0.45
2:B:962:GLU:CG	2:B:963:VAL:H	2.26	0.45
1:A:190:ARG:C	1:A:192:THR:H	2.20	0.45
1:A:18:ARG:HH11	1:A:612:LEU:HD22	1.76	0.45
1:A:609:ARG:CG	1:A:609:ARG:HH11	2.27	0.45
2:B:919:ILE:HG23	2:B:932:LEU:HD23	1.97	0.45
1:A:45:LEU:CD1	1:A:451:LEU:HD13	2.46	0.45
1:A:402:PHE:N	1:A:402:PHE:CD1	2.85	0.45
2:B:1009:LYS:CG	2:B:1016:SER:HB3	2.47	0.45
2:B:1009:LYS:HG2	2:B:1016:SER:HB3	1.97	0.45
2:B:726:LYS:HD3	2:B:876:THR:HG23	1.98	0.45
2:B:267:SER:HA	2:B:908:ARG:HH21	1.82	0.45
2:B:726:LYS:HD3	2:B:876:THR:CG2	2.47	0.45
1:A:467:HIS:O	1:A:470:PRO:HD3	2.17	0.45
1:A:672:TYR:HD2	1:A:678:TYR:CE2	2.34	0.45
2:B:979:GLN:NE2	2:B:985:SER:HA	2.31	0.45
2:B:409:ARG:C	2:B:411:ASP:H	2.20	0.45
1:A:174:GLN:HG2	1:A:188:VAL:HG22	1.99	0.45
2:B:633:VAL:CG1	2:B:651:VAL:HG12	2.46	0.45
2:B:655:THR:O	2:B:720:ALA:HB3	2.17	0.45
2:B:279:ARG:CZ	2:B:294:PRO:HG3	2.47	0.45
2:B:958:THR:HG21	2:B:989:THR:HA	1.99	0.45
2:B:958:THR:HG23	2:B:990:ILE:HG13	1.98	0.45
2:B:499:ASN:HA	2:B:525:GLY:O	2.16	0.45
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.82	0.45
1:A:644:ALA:O	1:A:663:THR:HB	2.17	0.45
1:A:78:TYR:CD2	1:A:101:ILE:HG12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:ALA:C	2:B:573:ASP:H	2.20	0.45
2:B:267:SER:HB2	2:B:908:ARG:HH21	1.81	0.44
2:B:312:PHE:CE1	2:B:344:ILE:HD11	2.51	0.44
1:A:190:ARG:CB	1:A:192:THR:HG22	2.46	0.44
2:B:974:ILE:HG13	2:B:975:MET:N	2.31	0.44
2:B:665:PHE:CD1	2:B:670:ASP:HB2	2.53	0.44
2:B:585:LEU:HD21	2:B:594:LEU:CB	2.46	0.44
1:A:153:MET:SD	1:A:387:GLN:HB3	2.57	0.44
2:B:618:VAL:HG23	2:B:619:TYR:N	2.32	0.44
1:A:178:LEU:C	1:A:180:CYS:H	2.20	0.44
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.45	0.44
2:B:747:GLN:HG3	2:B:765:ASN:OD1	2.17	0.44
2:B:992:LYS:CB	2:B:996:GLN:HG3	2.47	0.44
1:A:618:MET:CE	1:A:653:PHE:CD2	3.00	0.44
2:B:644:ASP:OD2	2:B:647:SER:HB2	2.16	0.44
1:A:12:GLU:OE1	1:A:18:ARG:HD2	2.17	0.44
2:B:455:LYS:C	2:B:457:GLY:H	2.20	0.44
2:B:642:TYR:CZ	2:B:644:ASP:HB2	2.52	0.44
1:A:183:ILE:HD12	2:B:547:MET:SD	2.57	0.44
1:A:147:LEU:HG	1:A:151:MET:HE2	2.00	0.44
2:B:739:SER:C	2:B:741:ASP:N	2.71	0.44
2:B:329:GLN:O	2:B:816:HIS:HE1	2.00	0.44
2:B:289:ARG:O	2:B:291:GLN:N	2.48	0.44
2:B:690:ALA:HB2	2:B:752:TYR:CB	2.48	0.44
2:B:339:LYS:HD2	2:B:342:ALA:CB	2.48	0.44
2:B:612:PHE:O	2:B:646:ALA:HB1	2.18	0.44
1:A:132:LEU:HD12	1:A:165:GLY:O	2.18	0.44
1:A:259:ARG:HG3	1:A:306:LEU:HD23	1.99	0.44
2:B:469:MET:HE1	2:B:678:LEU:HG	1.99	0.44
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.33	0.44
2:B:955:THR:HG23	2:B:990:ILE:O	2.18	0.44
1:A:648:LEU:O	1:A:658:ILE:HA	2.18	0.44
2:B:653:GLN:HE21	2:B:708:GLY:HA2	1.82	0.44
1:A:317:ASP:C	1:A:319:ASP:H	2.22	0.44
2:B:543:GLN:HB3	2:B:547:MET:HE1	2.00	0.43
2:B:706:PHE:CE2	2:B:793:SER:HA	2.52	0.43
1:A:23:VAL:HG12	1:A:513:ILE:HG12	2.00	0.43
2:B:1030:GLN:O	2:B:1032:LEU:N	2.47	0.43
1:A:511:GLN:N	1:A:511:GLN:CD	2.67	0.43
1:A:743:LEU:O	1:A:755:HIS:ND1	2.52	0.43
2:B:317:THR:HG21	2:B:319:CYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1025:HIS:O	2:B:1028:ILE:HG22	2.19	0.43
2:B:859:ARG:O	2:B:861:GLU:N	2.51	0.43
2:B:627:VAL:HG21	2:B:710:LEU:HD23	1.99	0.43
2:B:979:GLN:HE22	2:B:986:MET:H	1.67	0.43
1:A:543:LEU:HD11	1:A:591:GLN:HE22	1.84	0.43
1:A:519:GLN:OE1	1:A:576:LEU:HB2	2.16	0.43
1:A:392:LYS:HD3	1:A:396:GLY:HA2	2.00	0.43
1:A:6:GLU:O	1:A:10:GLN:HG3	2.18	0.43
2:B:988:LEU:HD12	2:B:989:THR:H	1.83	0.43
1:A:79:ARG:O	1:A:80:ALA:HB2	2.18	0.43
2:B:704:ASP:HB3	2:B:731:GLU:HB3	1.99	0.43
2:B:833:GLN:HB3	3:C:117:THR:CG2	2.49	0.43
1:A:747:VAL:HG12	1:A:748:SER:N	2.21	0.43
1:A:208:LYS:O	1:A:209:VAL:CB	2.66	0.43
2:B:955:THR:C	2:B:957:MET:N	2.72	0.43
2:B:902:MET:O	2:B:903:LEU:HB3	2.19	0.43
1:A:179:GLY:O	1:A:181:GLU:N	2.51	0.43
1:A:464:VAL:O	1:A:465:ASN:HB2	2.18	0.43
1:A:376:SER:O	1:A:379:THR:HG23	2.18	0.43
1:A:48:ARG:HH11	1:A:48:ARG:HG3	1.84	0.43
1:A:403:GLY:HA2	1:A:449:CYS:HA	2.01	0.43
1:A:547:ASP:OD2	1:A:743:LEU:HB3	2.18	0.43
2:B:854:CYS:O	2:B:867:ARG:CD	2.66	0.43
1:A:165:GLY:HA3	1:A:230:LEU:HD23	2.01	0.43
1:A:631:PRO:O	1:A:633:GLU:HG3	2.19	0.43
1:A:633:GLU:O	1:A:635:VAL:HG13	2.19	0.43
1:A:320:ASN:HA	1:A:320:ASN:HD22	1.63	0.43
1:A:577:TYR:N	1:A:578:PRO:CD	2.82	0.42
2:B:364:CYS:O	2:B:368:LYS:HA	2.18	0.42
1:A:678:TYR:N	1:A:678:TYR:CD1	2.87	0.42
1:A:173:VAL:HG11	1:A:270:ILE:HD12	2.01	0.42
2:B:936:SER:HB3	2:B:941:ILE:HD11	2.00	0.42
2:B:494:VAL:HG21	2:B:513:THR:HG22	2.01	0.42
1:A:59:VAL:C	1:A:60:LEU:HD23	2.40	0.42
2:B:272:ILE:HG23	2:B:297:THR:HB	2.00	0.42
2:B:603:VAL:O	2:B:604:ASN:CG	2.58	0.42
2:B:766:LEU:HD23	2:B:768:LEU:HD21	2.01	0.42
2:B:267:SER:CA	2:B:908:ARG:HH21	2.32	0.42
1:A:672:TYR:HD1	1:A:672:TYR:H	1.67	0.42
2:B:562:ILE:HB	2:B:622:LEU:HD21	2.01	0.42
2:B:384:TYR:CD1	2:B:384:TYR:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:676:ASN:O	2:B:680:ASN:HB2	2.20	0.42
1:A:98:TYR:O	1:A:99:ALA:C	2.58	0.42
1:A:255:PRO:HG2	1:A:258:LYS:CG	2.48	0.42
1:A:508:THR:C	1:A:509:GLN:HG2	2.39	0.42
1:A:183:ILE:CD1	2:B:509:MET:HE3	2.49	0.42
1:A:79:ARG:NH1	1:A:79:ARG:HG3	2.33	0.42
1:A:609:ARG:NH1	1:A:609:ARG:CG	2.82	0.42
1:A:58:PRO:O	1:A:59:VAL:CB	2.65	0.42
2:B:854:CYS:HB2	2:B:862:ILE:HG21	2.00	0.42
2:B:901:THR:HB	2:B:973:MET:CE	2.49	0.42
1:A:406:LEU:O	1:A:445:GLN:HA	2.20	0.42
2:B:271:VAL:HG21	2:B:842:VAL:HG23	2.00	0.42
2:B:475:LYS:O	2:B:475:LYS:HD2	2.20	0.42
2:B:415:LYS:HE2	5:B:1155:HOH:O	2.19	0.42
2:B:354:VAL:CG2	2:B:416:PRO:HG2	2.49	0.42
1:A:339:ALA:O	1:A:447:LYS:CE	2.68	0.42
2:B:709:ILE:HG22	2:B:719:MET:HG2	2.02	0.42
2:B:795:PHE:HB3	2:B:875:MET:CE	2.48	0.42
2:B:739:SER:OG	2:B:742:SER:HB2	2.20	0.42
2:B:523:LEU:HD23	5:B:1109:HOH:O	2.19	0.42
2:B:945:PHE:CD1	2:B:945:PHE:N	2.88	0.42
2:B:486:VAL:O	2:B:527:LEU:HA	2.19	0.42
2:B:439:ASN:HB3	2:B:440:PRO:HD2	2.01	0.42
2:B:992:LYS:O	2:B:996:GLN:HB2	2.19	0.42
2:B:1029:CYS:O	2:B:1032:LEU:HA	2.20	0.42
2:B:723:ASP:OD1	2:B:726:LYS:HG2	2.20	0.42
1:A:744:THR:HG21	1:A:752:PHE:CD1	2.54	0.42
1:A:536:THR:CG2	1:A:537:GLU:N	2.83	0.42
2:B:509:MET:HE1	2:B:547:MET:SD	2.60	0.42
1:A:420:ILE:HD13	1:A:532:TYR:HB2	2.02	0.42
2:B:316:THR:HA	2:B:785:ALA:HB3	2.01	0.42
1:A:153:MET:CE	1:A:154:SER:HA	2.49	0.41
2:B:838:ASP:OD1	2:B:841:LYS:HE3	2.20	0.41
1:A:687:ALA:HB3	1:A:688:PRO:CD	2.49	0.41
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.77	0.41
2:B:1025:HIS:ND1	3:C:120:MET:HG3	2.35	0.41
2:B:454:ILE:HD13	2:B:459:VAL:CG2	2.42	0.41
2:B:709:ILE:HD12	2:B:717:VAL:HG13	2.02	0.41
2:B:700:PHE:CZ	2:B:744:ALA:HB1	2.54	0.41
1:A:87:PHE:CZ	1:A:480:GLN:HB2	2.55	0.41
2:B:665:PHE:HE2	2:B:667:MET:CE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:PRO:HA	2:B:563:GLN:HB3	2.02	0.41
1:A:323:TYR:O	1:A:324:VAL:C	2.59	0.41
2:B:713:ASN:HD22	2:B:715:THR:H	1.66	0.41
2:B:964:GLY:HA3	2:B:968:SER:CB	2.50	0.41
2:B:617:ASN:OD1	2:B:617:ASN:O	2.38	0.41
2:B:411:ASP:O	2:B:412:HIS:C	2.58	0.41
1:A:134:VAL:HG11	1:A:288:MET:HE3	2.01	0.41
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.34	0.41
2:B:409:ARG:C	2:B:411:ASP:N	2.73	0.41
1:A:78:TYR:CD2	1:A:102:SER:HA	2.56	0.41
2:B:696:THR:HB	2:B:700:PHE:CZ	2.55	0.41
2:B:624:LYS:HE2	2:B:624:LYS:HB3	1.88	0.41
1:A:426:LEU:HD21	1:A:447:LYS:HB2	2.03	0.41
1:A:526:MET:HG3	1:A:577:TYR:OH	2.20	0.41
2:B:932:LEU:HD11	2:B:945:PHE:CZ	2.55	0.41
2:B:377:PHE:CD2	2:B:409:ARG:HD2	2.55	0.41
1:A:414:ILE:HG22	1:A:415:LYS:N	2.35	0.41
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.55	0.41
2:B:441:PRO:HA	2:B:575:PRO:O	2.21	0.41
1:A:394:MET:SD	1:A:394:MET:N	2.84	0.41
1:A:297:GLY:HA2	1:A:298:PRO:O	2.21	0.41
2:B:486:VAL:HG12	2:B:487:GLY:N	2.36	0.41
2:B:820:CYS:HA	2:B:823:LYS:HE2	2.03	0.41
2:B:643:VAL:CG1	2:B:648:LEU:HD12	2.50	0.41
2:B:356:HIS:CD2	2:B:362:VAL:HG23	2.56	0.41
2:B:707:GLY:O	2:B:709:ILE:HG12	2.21	0.41
2:B:458:LEU:HD12	2:B:461:LEU:HD23	2.03	0.41
2:B:529:ASN:HD22	2:B:529:ASN:C	2.24	0.41
2:B:441:PRO:HB3	2:B:575:PRO:HG2	2.02	0.41
2:B:536:VAL:O	2:B:539:ASN:HB3	2.21	0.41
1:A:289:PHE:CD1	1:A:289:PHE:N	2.89	0.41
2:B:469:MET:CE	2:B:682:ILE:HD12	2.50	0.41
1:A:15:ASP:O	1:A:16:GLY:C	2.59	0.41
1:A:154:SER:O	1:A:158:LEU:HG	2.21	0.40
1:A:612:LEU:HD23	1:A:613:THR:N	2.36	0.40
1:A:623:LEU:HG	1:A:648:LEU:HD22	2.04	0.40
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.56	0.40
2:B:464:GLU:HA	2:B:467:LYS:HE3	2.03	0.40
2:B:857:LEU:HA	2:B:857:LEU:HD12	1.68	0.40
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.83	0.40
1:A:155:LEU:CD2	1:A:240:LEU:HD13	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:933:GLY:HA2	2:B:993:GLN:HB2	2.04	0.40
2:B:332:ILE:HD12	2:B:777:LEU:HD13	2.02	0.40
2:B:937:PRO:HG2	2:B:940:LEU:HD12	2.02	0.40
1:A:555:GLN:HG2	1:A:760:ALA:O	2.21	0.40
1:A:283:GLY:CA	1:A:486:GLN:HE22	2.33	0.40
1:A:153:MET:CE	1:A:157:LEU:CD1	3.00	0.40
2:B:602:LEU:HD21	2:B:859:ARG:HD3	2.02	0.40
2:B:401:GLN:HG3	2:B:411:ASP:OD2	2.21	0.40
1:A:537:GLU:HG3	1:A:537:GLU:H	1.75	0.40
1:A:376:SER:OG	1:A:379:THR:HG23	2.22	0.40
2:B:268:PRO:O	2:B:272:ILE:HG13	2.22	0.40
1:A:189:PHE:N	1:A:189:PHE:CD1	2.88	0.40
1:A:268:LEU:HD22	1:A:272:VAL:HG23	2.03	0.40
2:B:289:ARG:HD3	2:B:768:LEU:O	2.20	0.40
1:A:54:ILE:HD12	1:A:56:TYR:CE2	2.56	0.40
2:B:649:GLY:HA2	2:B:652:PRO:CG	2.52	0.40
2:B:738:LEU:HB2	2:B:770:CYS:SG	2.61	0.40
2:B:854:CYS:HB3	2:B:862:ILE:CD1	2.49	0.40
1:A:546:LEU:HD21	1:A:584:LEU:CD2	2.52	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	720/764 (94%)	618 (86%)	76 (11%)	26 (4%)	4	24
2	B	763/770 (99%)	651 (85%)	76 (10%)	36 (5%)	3	17
3	C	4/7 (57%)	4 (100%)	0	0	100	100
All	All	1487/1541 (96%)	1273 (86%)	152 (10%)	62 (4%)	3	20

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	80	ALA
1	A	237	ASP
1	A	465	ASN
1	A	466	GLN
1	A	467	HIS
1	A	468	ASN
1	A	593	PHE
2	B	289	ARG
2	B	304	ASP
2	B	412	HIS
2	B	492	ASN
2	B	503	ASN
2	B	527	LEU
2	B	603	VAL
2	B	604	ASN
2	B	899	LYS
2	B	900	SER
2	B	902	MET
2	B	964	GLY
2	B	993	GLN
2	B	996	GLN
2	B	998	GLU
2	B	1032	LEU
1	A	180	CYS
1	A	297	GLY
1	A	324	VAL
1	A	537	GLU
1	A	575	SER
1	A	610	GLN
1	A	746	ASP
2	B	597	ARG
2	B	862	ILE
2	B	956	ASP
2	B	995	GLU
1	A	99	ALA
1	A	536	THR
1	A	700	PHE
1	A	744	THR
2	B	397	PRO
2	B	413	TYR
2	B	429	LEU
2	B	860	PRO

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Mol	Chain	Res	Type
1	A	59	VAL
1	A	184	SER
2	B	398	PHE
2	B	423	TYR
2	B	861	GLU
2	B	903	LEU
2	B	961	PRO
2	B	963	VAL
2	B	980	GLN
1	A	116	SER
2	B	859	ARG
2	B	966	PRO
1	A	109	GLU
1	A	469	ALA
1	A	470	PRO
2	B	524	ASP
1	A	540	PRO
2	B	290	GLY
2	B	1006	VAL

### 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	635/666 (95%)	598 (94%)	37 (6%)	25	63
2	B	680/682 (100%)	642 (94%)	38 (6%)	26	65
3	C	6/7 (86%)	6 (100%)	0	100	100
All	All	1321/1355 (98%)	1246 (94%)	75 (6%)	25	64

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	34	MET
1	A	41	LEU

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Mol	Chain	Res	Type
1	A	67	ARG
1	A	105	ASN
1	A	109	GLU
1	A	116	SER
1	A	141	ASP
1	A	153	MET
1	A	194	ASP
1	A	237	ASP
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	311	ARG
1	A	313	TRP
1	A	320	ASN
1	A	332	GLU
1	A	362	CYS
1	A	376	SER
1	A	394	MET
1	A	451	LEU
1	A	468	ASN
1	A	470	PRO
1	A	476	ARG
1	A	491	GLN
1	A	498	THR
1	A	528	ARG
1	A	570	PHE
1	A	615	SER
1	A	637	LEU
1	A	652	THR
1	A	673	GLN
1	A	677	GLU
1	A	690	ASP
1	A	695	ILE
1	A	696	LEU
2	B	267	SER
2	B	313	ILE
2	B	334	LEU
2	B	355	ASN
2	B	376	GLN
2	B	383	ARG
2	B	391	CYS
2	B	401	GLN

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Mol	Chain	Res	Type
2	B	409	ARG
2	B	411	ASP
2	B	446	MET
2	B	470	LEU
2	B	475	LYS
2	B	494	VAL
2	B	518	VAL
2	B	523	LEU
2	B	528	VAL
2	B	529	ASN
2	B	553	GLU
2	B	566	MET
2	B	585	LEU
2	B	599	ASP
2	B	620	ASP
2	B	633	VAL
2	B	647	SER
2	B	653	GLN
2	B	661	LYS
2	B	691	ILE
2	B	713	ASN
2	B	777	LEU
2	B	799	LEU
2	B	807	ARG
2	B	834	LEU
2	B	876	THR
2	B	896	LEU
2	B	921	LEU
2	B	946	ASN
2	B	1027	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	296	GLN
1	A	320	ASN
1	A	330	HIS
1	A	397	GLN
1	A	436	ASN
1	A	468	ASN
1	A	486	GLN

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Mol	Chain	Res	Type
1	A	511	GLN
1	A	549	GLN
1	A	579	GLN
1	A	583	HIS
1	A	591	GLN
1	A	595	ASN
1	A	614	GLN
1	A	673	GLN
1	A	710	HIS
2	B	347	ASN
2	B	355	ASN
2	B	356	HIS
2	B	365	ASN
2	B	385	GLN
2	B	492	ASN
2	B	503	ASN
2	B	508	GLN
2	B	529	ASN
2	B	615	GLN
2	B	617	ASN
2	B	653	GLN
2	B	663	ASN
2	B	666	GLN
2	B	668	HIS
2	B	713	ASN
2	B	734	HIS
2	B	813	GLN
2	B	816	HIS
2	B	853	ASN
2	B	942	GLN
2	B	946	ASN
2	B	969	GLN
2	B	970	GLN
2	B	979	GLN
2	B	996	GLN
2	B	1003	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	726/764 (95%)	-0.48	5 (0%) 89 70	21, 48, 92, 144	0
2	B	767/770 (99%)	-0.45	3 (0%) 93 80	22, 50, 102, 128	0
3	C	6/7 (85%)	0.35	0 100 100	59, 77, 90, 108	0
All	All	1499/1541 (97%)	-0.46	8 (0%) 91 76	21, 49, 98, 144	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1033	ASN	3.8
1	A	469	ALA	3.2
2	B	604	ASN	2.8
1	A	467	HIS	2.5
2	B	2	MET	2.5
1	A	468	ASN	2.3
1	A	471	ILE	2.2
1	A	30	GLU	2.1

### 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	ZN	B	1100	1/1	0.98	0.14	-0.35	57,57,57,57	0
4	ZN	A	800	1/1	0.99	0.10	-1.16	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.