



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:47 PM GMT

PDB ID : 1M2V  
Title : Crystal Structure of the yeast Sec23/24 heterodimer  
Authors : Bi, X.; Corpina, R.A.; Goldberg, J.  
Deposited on : 2002-06-25  
Resolution : 2.75 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

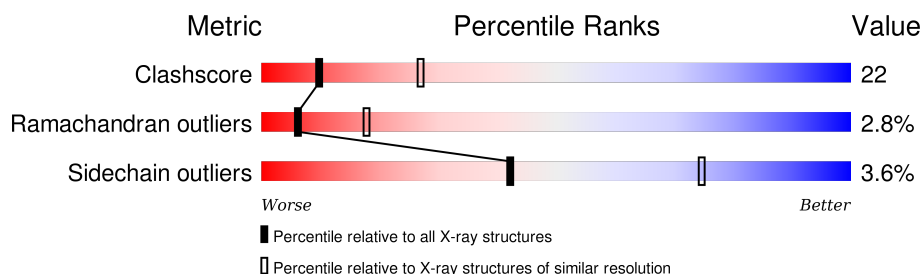
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	768	 55% 34% • 8%
2	B	926	 46% 32% • 19%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11577 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 SEC23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	0	0
			5574	3560	933	1059	22			

- Molecule 2 is a protein called protein transport protein SEC24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	748	Total	C	N	O	S	0	0	0
			5932	3772	1018	1104	38			

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	35	Total	O	0	0
			35	35		



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.31 Å   126.37 Å   180.20 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.96 – 2.75	Depositor
% Data completeness (in resolution range)	91.2 (19.96-2.75)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

## 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	0.40	0/5706	0.66	1/7765 (0.0%)
2	B	0.39	0/6054	0.67	1/8214 (0.0%)
All	All	0.39	0/11760	0.66	2/15979 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	GLY	N-CA-C	6.93	130.42	113.10
2	B	768	LEU	CA-CB-CG	5.33	127.57	115.30

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	5574	0	5475	230	0
2	B	5932	0	5958	282	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	34	0	0	5	0
4	B	35	0	0	3	0
All	All	11577	0	11433	510	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 22.

All (510) 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:907:ILE:HG22	2:B:908:LEU:HG	1.35	1.08
2:B:147:LEU:HB3	2:B:148:PRO:HD2	1.16	1.08
2:B:147:LEU:CB	2:B:148:PRO:HD2	1.97	0.95
1:A:651:ASN:H	1:A:651:ASN:HD22	0.96	0.94
1:A:359:LYS:HD2	1:A:607:ALA:HB1	1.49	0.92
1:A:669:GLN:HE21	1:A:669:GLN:HA	1.33	0.92
1:A:399:ALA:HB3	1:A:450:LEU:HD13	1.52	0.90
2:B:441:LYS:HE2	2:B:498:ASP:OD2	1.72	0.89
2:B:147:LEU:HB3	2:B:148:PRO:CD	2.02	0.88
2:B:459:ARG:HH11	2:B:459:ARG:HG2	1.39	0.87
2:B:375:MET:HE1	2:B:413:ILE:HG21	1.57	0.86
1:A:379:ILE:HD12	1:A:379:ILE:H	1.42	0.84
2:B:333:LEU:HB2	2:B:400:ARG:NH2	1.93	0.83
2:B:352:ASN:HD22	2:B:353:ALA:N	1.75	0.82
1:A:651:ASN:H	1:A:651:ASN:ND2	1.75	0.82
1:A:70:VAL:HB	1:A:79:SER:HB2	1.59	0.82
1:A:485:ALA:HB2	1:A:511:LEU:HD11	1.60	0.81
1:A:119:THR:HG21	1:A:280:ILE:HD12	1.61	0.80
2:B:147:LEU:HD13	2:B:914:ARG:NH1	1.97	0.79
1:A:157:ILE:HG21	1:A:238:LEU:HD11	1.65	0.79
2:B:147:LEU:O	2:B:148:PRO:C	2.21	0.79
1:A:550:ARG:CD	1:A:554:ARG:HH21	1.95	0.79
2:B:680:GLN:HG3	2:B:920:MET:HE1	1.65	0.78
1:A:96:LEU:HD22	1:A:102:PRO:HD3	1.65	0.77
2:B:919:ILE:O	2:B:923:ARG:HG3	1.83	0.77
2:B:296:TYR:O	2:B:624:ARG:NH1	2.19	0.76
1:A:703:VAL:O	1:A:704:ASP:HB2	1.85	0.76
1:A:651:ASN:N	1:A:651:ASN:HD22	1.78	0.76
1:A:750:VAL:HG12	1:A:751:SER:H	1.49	0.76
1:A:15:THR:HG22	1:A:528:ALA:HA	1.68	0.75
1:A:239:ASN:O	1:A:243:GLU:HG3	1.87	0.75
2:B:660:VAL:HG11	2:B:741:GLU:HB3	1.68	0.74
2:B:709:MET:HE1	2:B:712:LEU:HD23	1.69	0.74
2:B:142:ASP:CG	2:B:700:PRO:HB3	2.08	0.73
1:A:432:ILE:HD13	1:A:442:THR:HA	1.69	0.73
2:B:567:ARG:HH21	2:B:599:ASN:HD22	1.36	0.72
1:A:665:TYR:OH	1:A:716:ALA:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:GLY:O	2:B:293:PRO:HG3	1.90	0.72
2:B:557:VAL:HG13	2:B:582:LEU:HD11	1.70	0.71
2:B:225:ASP:OD1	2:B:227:LEU:HB3	1.90	0.71
1:A:688:LYS:O	1:A:692:GLU:HG2	1.91	0.71
2:B:142:ASP:O	2:B:146:GLU:HG2	1.91	0.70
1:A:403:ASN:HB3	1:A:492:THR:HG23	1.74	0.70
2:B:696:ALA:HB2	2:B:702:ARG:HH21	1.57	0.70
2:B:801:LEU:HD11	2:B:808:LEU:HD22	1.74	0.70
2:B:493:VAL:HG23	2:B:495:ILE:HG13	1.73	0.70
1:A:557:ILE:O	1:A:561:GLN:HG3	1.92	0.69
2:B:154:LEU:HG	2:B:709:MET:HE2	1.74	0.69
1:A:681:ASP:HB3	1:A:684:TYR:HD1	1.55	0.69
2:B:699:ALA:HB1	2:B:921:LYS:NZ	2.08	0.69
1:A:669:GLN:HE21	1:A:669:GLN:CA	2.04	0.69
2:B:279:ASP:HA	2:B:284:LYS:HE3	1.74	0.69
1:A:80:CYS:O	1:A:84:ASN:HA	1.93	0.69
1:A:30:VAL:HG22	1:A:558:LYS:HD3	1.74	0.68
2:B:768:LEU:HG	2:B:769:PRO:HD2	1.73	0.68
1:A:550:ARG:CG	1:A:554:ARG:HH21	2.07	0.68
1:A:102:PRO:HD2	1:A:105:LEU:HD12	1.75	0.68
2:B:459:ARG:NH1	2:B:459:ARG:HG2	2.07	0.67
1:A:395:TYR:CD2	1:A:497:SER:HA	2.29	0.67
2:B:766:ALA:O	2:B:768:LEU:N	2.26	0.67
2:B:764:ASP:HA	2:B:851:ARG:HH22	1.60	0.67
1:A:669:GLN:NE2	1:A:669:GLN:HA	2.09	0.67
2:B:312:VAL:HG11	2:B:414:PHE:CD2	2.30	0.67
1:A:359:LYS:HD2	1:A:607:ALA:CB	2.25	0.66
2:B:303:PRO:HG3	2:B:342:ARG:CZ	2.25	0.66
1:A:512:LEU:HD13	1:A:516:THR:HG21	1.77	0.66
1:A:74:ARG:HG3	1:A:75:ASN:H	1.61	0.66
2:B:312:VAL:HG11	2:B:414:PHE:CG	2.31	0.66
2:B:362:ASP:OD1	2:B:401:GLN:HB2	1.95	0.65
2:B:812:MET:SD	2:B:820:LEU:HD22	2.36	0.65
2:B:750:LYS:HE3	2:B:805:GLY:HA2	1.77	0.65
2:B:399:CYS:O	2:B:403:ILE:HG13	1.97	0.65
2:B:672:ARG:HH11	2:B:725:SER:HB3	1.62	0.65
2:B:297:THR:HG22	2:B:624:ARG:HD3	1.79	0.65
2:B:422:PHE:H	2:B:451:ASN:HB3	1.61	0.65
2:B:525:PHE:CE2	2:B:527:PRO:HG3	2.33	0.64
2:B:920:MET:HA	2:B:920:MET:HE3	1.79	0.64
1:A:616:GLU:HG3	1:A:620:ASN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:PRO:O	2:B:151:ILE:HG12	1.97	0.64
1:A:171:LEU:HA	1:A:237:LYS:HE2	1.80	0.64
1:A:541:GLU:OE1	1:A:610:ARG:HD3	1.98	0.64
2:B:856:ILE:HD13	2:B:871:LEU:HD22	1.79	0.64
1:A:671:ALA:O	1:A:675:LYS:HB2	1.96	0.64
1:A:699:ALA:O	1:A:703:VAL:HG23	1.98	0.64
2:B:817:VAL:C	2:B:819:ALA:H	2.01	0.64
2:B:818:PRO:C	2:B:820:LEU:H	2.00	0.64
2:B:914:ARG:O	2:B:918:GLN:HG2	1.98	0.64
1:A:612:ILE:HG12	4:A:826:HOH:O	1.97	0.64
2:B:789:ALA:O	2:B:904:GLU:HB2	1.98	0.64
2:B:147:LEU:HD13	2:B:914:ARG:HH12	1.61	0.63
1:A:450:LEU:N	1:A:450:LEU:HD12	2.12	0.63
2:B:255:PHE:CZ	2:B:612:GLN:HB2	2.33	0.63
1:A:379:ILE:HD12	1:A:379:ILE:N	2.10	0.63
2:B:312:VAL:O	2:B:312:VAL:HG12	1.99	0.63
1:A:278:LYS:HE3	1:A:339:ASN:ND2	2.14	0.62
2:B:680:GLN:CG	2:B:920:MET:HE1	2.28	0.62
2:B:750:LYS:HD2	2:B:803:ASP:OD2	1.98	0.62
2:B:352:ASN:HD22	2:B:353:ALA:H	1.47	0.62
1:A:379:ILE:H	1:A:379:ILE:CD1	2.10	0.62
1:A:132:SER:HB3	1:A:289:SER:OG	2.00	0.62
2:B:808:LEU:O	2:B:871:LEU:HD12	1.98	0.61
2:B:449:LEU:HD12	2:B:450:PRO:HD2	1.81	0.61
2:B:539:LYS:HA	2:B:868:TYR:CD2	2.34	0.61
1:A:550:ARG:HG2	1:A:554:ARG:HH21	1.66	0.61
1:A:767:GLN:HB3	4:A:815:HOH:O	2.01	0.61
1:A:225:ASN:OD1	1:A:276:CYS:HB2	2.00	0.61
2:B:424:LEU:HG	2:B:428:LEU:HD22	1.81	0.61
1:A:250:TRP:CE3	2:B:389:PRO:HB3	2.36	0.60
2:B:668:LEU:HG	2:B:672:ARG:HH21	1.67	0.60
2:B:209:PRO:HG3	2:B:558:MET:HE1	1.82	0.60
2:B:539:LYS:HE3	2:B:543:GLU:OE2	2.02	0.60
2:B:687:LYS:NZ	2:B:925:SER:HA	2.15	0.60
2:B:524:HIS:CE1	2:B:866:ILE:HD11	2.37	0.60
2:B:209:PRO:HG3	2:B:558:MET:CE	2.32	0.60
1:A:182:PHE:HZ	1:A:197:LEU:HD21	1.67	0.59
1:A:653:ILE:HD11	1:A:691:LEU:HD23	1.83	0.59
2:B:270:ASP:HB2	2:B:273:ASP:HB3	1.83	0.59
1:A:114:THR:O	1:A:115:ASN:O	2.21	0.59
2:B:205:LEU:HD13	2:B:611:VAL:HG11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HB2	2:B:400:ARG:CZ	2.32	0.59
2:B:352:ASN:ND2	2:B:353:ALA:N	2.49	0.59
2:B:133:ARG:NH2	2:B:635:THR:O	2.36	0.59
2:B:915:GLU:O	2:B:919:ILE:HG13	2.02	0.59
2:B:711:PRO:HD2	4:B:976:HOH:O	2.00	0.59
1:A:157:ILE:HG21	1:A:238:LEU:CD1	2.32	0.59
1:A:417:LEU:HD23	1:A:418:ILE:N	2.18	0.59
2:B:667:SER:HB3	2:B:670:ASP:HB2	1.85	0.59
2:B:764:ASP:HA	2:B:851:ARG:NH2	2.17	0.59
1:A:525:GLN:OE1	1:A:582:LEU:HB2	2.03	0.59
1:A:330:ASN:O	1:A:334:GLN:HG3	2.03	0.58
1:A:74:ARG:HG3	1:A:75:ASN:N	2.16	0.58
2:B:272:ASN:O	2:B:274:PRO:HD3	2.04	0.58
2:B:728:VAL:HG21	2:B:733:ARG:NH2	2.18	0.58
2:B:228:ILE:HD13	2:B:290:TYR:CD2	2.38	0.58
2:B:147:LEU:CB	2:B:148:PRO:CD	2.74	0.58
2:B:135:MET:HE2	2:B:641:GLU:OE1	2.03	0.58
2:B:729:PRO:HB2	2:B:732:HIS:HD2	1.68	0.58
2:B:378:ILE:HD11	2:B:387:PRO:HG3	1.86	0.58
1:A:703:VAL:O	1:A:704:ASP:CB	2.50	0.57
2:B:593:SER:HB2	2:B:744:PRO:HA	1.86	0.57
2:B:872:TYR:CE2	2:B:897:TRP:HZ3	2.23	0.57
2:B:849:ASN:OD1	2:B:853:ARG:HD3	2.04	0.57
1:A:557:ILE:HD13	1:A:762:VAL:HG11	1.86	0.57
2:B:563:SER:HB3	2:B:610:TYR:H	1.68	0.57
2:B:672:ARG:NH1	2:B:725:SER:HB3	2.19	0.57
2:B:138:LEU:HD22	2:B:704:CYS:HB3	1.85	0.57
1:A:129:ASP:OD2	1:A:260:ARG:HD3	2.05	0.57
2:B:303:PRO:HG3	2:B:342:ARG:NH1	2.19	0.57
2:B:147:LEU:HD13	2:B:914:ARG:CZ	2.34	0.57
1:A:25:ASP:OD1	1:A:514:PHE:HB2	2.05	0.57
1:A:159:LEU:HG	1:A:169:HIS:HD2	1.69	0.57
2:B:696:ALA:CB	2:B:702:ARG:HH21	2.18	0.57
1:A:616:GLU:CG	1:A:620:ASN:HB2	2.35	0.56
1:A:61:CYS:SG	1:A:83:CYS:HB3	2.45	0.56
2:B:802:ILE:O	2:B:808:LEU:HD23	2.05	0.56
1:A:132:SER:HB3	1:A:289:SER:CB	2.35	0.56
1:A:659:PHE:O	1:A:709:PRO:HB3	2.06	0.56
1:A:347:ALA:HB2	1:A:353:ILE:HD13	1.87	0.56
2:B:225:ASP:HB3	4:B:984:HOH:O	2.06	0.56
1:A:166:VAL:HG22	1:A:182:PHE:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLU:HB3	1:A:622:LEU:HD11	1.87	0.55
2:B:677:LYS:HG2	2:B:681:ASP:OD2	2.07	0.55
2:B:375:MET:CE	2:B:413:ILE:HG21	2.31	0.55
2:B:809:PHE:CD2	2:B:898:ALA:HB2	2.42	0.55
1:A:131:THR:OG1	1:A:260:ARG:NH1	2.38	0.55
1:A:399:ALA:HB3	1:A:450:LEU:CD1	2.29	0.54
1:A:757:THR:O	1:A:761:GLN:HG3	2.07	0.54
1:A:240:GLN:O	1:A:244:ASN:ND2	2.40	0.54
2:B:801:LEU:HD12	2:B:809:PHE:O	2.07	0.54
2:B:822:PHE:CD1	2:B:822:PHE:N	2.74	0.54
2:B:162:VAL:O	2:B:634:PRO:HG3	2.08	0.54
2:B:488:ILE:HD11	2:B:578:ARG:HH22	1.71	0.54
1:A:681:ASP:HB3	1:A:684:TYR:CD1	2.39	0.54
1:A:327:LYS:O	1:A:331:GLN:HG3	2.07	0.54
2:B:216:ASP:O	2:B:219:PRO:HD3	2.07	0.54
2:B:277:ARG:O	2:B:279:ASP:N	2.41	0.54
1:A:120:VAL:HG21	1:A:277:TYR:CE2	2.43	0.54
1:A:420:HIS:CE1	1:A:615:ARG:HB2	2.43	0.54
2:B:410:ILE:HB	2:B:411:PRO:HD3	1.89	0.54
2:B:352:ASN:HA	2:B:452:LEU:HD23	1.90	0.54
2:B:361:LEU:HD22	2:B:398:ALA:HB1	1.90	0.54
1:A:224:LEU:HD22	1:A:272:LEU:CD1	2.38	0.54
2:B:191:LYS:HE3	2:B:604:ILE:O	2.08	0.54
2:B:146:GLU:O	2:B:147:LEU:O	2.26	0.54
1:A:528:ALA:O	1:A:532:MET:HG2	2.08	0.54
1:A:17:ASN:HB2	1:A:522:SER:HB2	1.90	0.54
1:A:132:SER:HB2	1:A:136:ASN:HD22	1.72	0.53
1:A:164:ASN:HB2	1:A:250:TRP:CD1	2.43	0.53
1:A:159:LEU:HG	1:A:169:HIS:CD2	2.43	0.53
1:A:432:ILE:CD1	1:A:442:THR:HA	2.37	0.53
2:B:429:LYS:HD2	2:B:454:ILE:CD1	2.38	0.53
1:A:42:GLU:OE2	1:A:397:LYS:HE2	2.09	0.53
2:B:601:ASP:OD1	2:B:602:GLU:N	2.41	0.53
1:A:612:ILE:HD12	1:A:660:PHE:CE2	2.43	0.53
2:B:496:THR:HA	2:B:519:THR:HB	1.89	0.53
2:B:699:ALA:N	2:B:700:PRO:HD3	2.24	0.53
2:B:250:ARG:HB3	2:B:260:ASN:O	2.09	0.53
2:B:819:ALA:HA	2:B:822:PHE:CE1	2.44	0.53
1:A:90:PRO:HG2	1:A:93:TYR:CD2	2.44	0.53
2:B:346:SER:OG	2:B:393:VAL:HG22	2.09	0.53
2:B:754:PRO:HG3	2:B:901:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:PRO:HG3	2:B:342:ARG:NH2	2.24	0.52
1:A:693:GLU:O	1:A:697:GLU:HG2	2.09	0.52
2:B:498:ASP:C	2:B:499:LEU:HD12	2.30	0.52
2:B:699:ALA:HB1	2:B:921:LYS:HZ1	1.74	0.52
2:B:822:PHE:HD1	2:B:822:PHE:N	2.08	0.52
1:A:71:ILE:O	1:A:73:PRO:HD3	2.09	0.52
2:B:142:ASP:OD2	2:B:700:PRO:HB3	2.08	0.52
2:B:406:LEU:O	2:B:410:ILE:HG13	2.10	0.52
1:A:550:ARG:HG3	1:A:550:ARG:HH11	1.74	0.52
2:B:533:ASN:HB3	2:B:536:ASP:OD2	2.10	0.52
1:A:591:ARG:HG3	1:A:591:ARG:HH11	1.75	0.52
1:A:417:LEU:C	1:A:417:LEU:HD23	2.30	0.52
1:A:48:VAL:HA	1:A:111:GLU:O	2.10	0.52
1:A:109:THR:HA	1:A:504:VAL:O	2.10	0.52
1:A:550:ARG:CD	1:A:554:ARG:NH2	2.71	0.52
2:B:715:HIS:HB2	2:B:916:PHE:CE2	2.45	0.52
2:B:722:ALA:HB1	2:B:737:LEU:HD23	1.92	0.52
1:A:574:PHE:CE2	1:A:576:LEU:HD22	2.44	0.52
2:B:680:GLN:CB	2:B:920:MET:HE1	2.40	0.51
1:A:403:ASN:HB3	1:A:492:THR:CG2	2.40	0.51
2:B:817:VAL:O	2:B:819:ALA:N	2.42	0.51
2:B:906:LYS:O	2:B:907:ILE:HD13	2.10	0.51
2:B:279:ASP:CA	2:B:284:LYS:HE3	2.39	0.51
2:B:420:THR:O	2:B:420:THR:HG22	2.10	0.51
1:A:550:ARG:HD3	1:A:554:ARG:HH21	1.74	0.51
1:A:235:GLU:O	1:A:239:ASN:HB2	2.11	0.51
2:B:162:VAL:O	2:B:163:ILE:HD13	2.10	0.51
2:B:519:THR:O	2:B:520:ALA:HB3	2.10	0.51
2:B:817:VAL:C	2:B:819:ALA:N	2.64	0.51
1:A:273:LEU:HB3	1:A:341:HIS:CE1	2.46	0.51
2:B:516:SER:HB2	2:B:521:GLY:C	2.31	0.51
1:A:366:GLY:HA3	1:A:449:SER:O	2.11	0.51
1:A:198:THR:HG22	1:A:222:PHE:O	2.11	0.51
2:B:722:ALA:HB1	2:B:737:LEU:CD2	2.41	0.51
2:B:704:CYS:SG	2:B:707:LEU:HD12	2.50	0.51
1:A:674:ARG:O	1:A:676:ALA:N	2.44	0.51
2:B:516:SER:HB2	2:B:522:GLN:N	2.26	0.50
2:B:860:ARG:HG2	2:B:869:GLN:HB2	1.93	0.50
2:B:417:ASN:OD1	2:B:419:ILE:N	2.41	0.50
2:B:250:ARG:HA	2:B:262:VAL:HG23	1.93	0.50
2:B:372:GLN:HG2	2:B:373:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:768:LEU:CG	2:B:769:PRO:HD2	2.40	0.50
2:B:448:THR:HG22	2:B:449:LEU:O	2.11	0.50
1:A:395:TYR:CE2	1:A:497:SER:HA	2.46	0.50
2:B:710:PHE:HB3	2:B:711:PRO:HD3	1.94	0.50
1:A:3:PHE:CE1	1:A:524:ASP:HA	2.46	0.50
1:A:707:PRO:HD3	4:A:826:HOH:O	2.12	0.50
2:B:248:GLY:O	2:B:277:ARG:NH2	2.33	0.50
1:A:94:THR:HG22	1:A:94:THR:O	2.12	0.50
2:B:715:HIS:CE1	2:B:719:LYS:HE3	2.46	0.50
1:A:120:VAL:HG21	1:A:277:TYR:HE2	1.76	0.50
1:A:97:SER:OG	1:A:99:GLU:HG2	2.12	0.50
2:B:499:LEU:HD12	2:B:499:LEU:N	2.27	0.49
1:A:550:ARG:HG2	1:A:554:ARG:HE	1.76	0.49
2:B:818:PRO:C	2:B:820:LEU:N	2.66	0.49
1:A:264:SER:O	1:A:268:ILE:HG12	2.12	0.49
1:A:371:LEU:O	1:A:710:ARG:NH2	2.44	0.49
2:B:504:GLU:OE2	2:B:530:SER:HB3	2.12	0.49
1:A:693:GLU:N	1:A:694:PRO:HD2	2.27	0.49
2:B:794:PHE:HA	2:B:800:TYR:CZ	2.48	0.49
1:A:615:ARG:NH1	4:A:826:HOH:O	2.45	0.49
1:A:664:ILE:HD12	1:A:711:PHE:CZ	2.47	0.49
1:A:725:LEU:C	1:A:727:LYS:H	2.16	0.49
1:A:53:PRO:HG3	1:A:112:TYR:CG	2.48	0.49
2:B:855:ILE:O	2:B:858:GLN:HB3	2.12	0.49
2:B:907:ILE:HG22	2:B:908:LEU:N	2.27	0.49
2:B:150:PRO:HG2	2:B:708:ARG:HH11	1.77	0.49
2:B:423:ALA:HA	2:B:452:LEU:O	2.13	0.49
2:B:589:PRO:O	2:B:590:ARG:HD3	2.13	0.49
2:B:911:GLU:HG3	2:B:919:ILE:HD11	1.94	0.49
1:A:39:PRO:HG3	1:A:404:MET:HE1	1.94	0.48
2:B:338:ASN:OD1	2:B:341:GLU:HA	2.13	0.48
1:A:23:ARG:HH21	1:A:461:GLU:CD	2.16	0.48
1:A:54:VAL:HG21	1:A:93:TYR:HE2	1.78	0.48
1:A:659:PHE:HA	1:A:705:ARG:NH1	2.29	0.48
2:B:667:SER:HB3	2:B:670:ASP:CB	2.44	0.48
1:A:110:ILE:HG12	1:A:111:GLU:N	2.29	0.48
2:B:356:TYR:OH	2:B:430:SER:HB3	2.13	0.48
1:A:484:LEU:HD23	1:A:510:GLN:HA	1.94	0.48
2:B:703:LEU:HG	2:B:704:CYS:H	1.78	0.48
2:B:488:ILE:HD11	2:B:578:ARG:NH2	2.28	0.48
2:B:215:ASP:O	2:B:219:PRO:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:764:ASP:CA	2:B:851:ARG:HH22	2.24	0.48
1:A:556:LEU:HD22	1:A:587:THR:HG21	1.95	0.48
1:A:664:ILE:HD12	1:A:711:PHE:HZ	1.78	0.48
1:A:286:LEU:HD12	1:A:287:PHE:N	2.28	0.48
2:B:796:ARG:NH1	2:B:815:ASP:OD2	2.47	0.48
2:B:352:ASN:N	2:B:352:ASN:HD22	2.11	0.48
2:B:312:VAL:CG1	2:B:312:VAL:O	2.61	0.48
1:A:624:MET:HG2	1:A:660:PHE:CE1	2.48	0.48
2:B:192:ASN:HA	2:B:603:SER:HA	1.96	0.48
2:B:230:ARG:HD3	2:B:237:TYR:CD2	2.49	0.47
2:B:795:GLU:C	2:B:797:TYR:H	2.17	0.47
1:A:251:SER:O	1:A:253:PRO:HD3	2.14	0.47
2:B:133:ARG:NE	2:B:135:MET:SD	2.87	0.47
2:B:168:MET:SD	2:B:175:SER:OG	2.69	0.47
2:B:534:PRO:O	2:B:538:VAL:HG23	2.13	0.47
1:A:612:ILE:HD12	1:A:660:PHE:HE2	1.79	0.47
2:B:715:HIS:NE2	2:B:719:LYS:HE3	2.30	0.47
2:B:795:GLU:HB3	2:B:797:TYR:CE2	2.49	0.47
1:A:542:THR:O	1:A:542:THR:HG22	2.15	0.47
1:A:759:LEU:O	1:A:759:LEU:HD12	2.15	0.47
2:B:135:MET:HE1	2:B:634:PRO:HB2	1.97	0.47
2:B:378:ILE:CD1	2:B:387:PRO:HG3	2.44	0.47
2:B:177:ALA:HB1	2:B:182:ILE:HG22	1.96	0.47
2:B:277:ARG:C	2:B:279:ASP:H	2.18	0.47
1:A:61:CYS:O	1:A:62:LYS:HB2	2.15	0.47
1:A:425:LYS:NZ	1:A:441:ALA:HB3	2.29	0.47
2:B:848:PHE:O	2:B:851:ARG:HB2	2.15	0.47
1:A:224:LEU:HD22	1:A:272:LEU:HD12	1.95	0.47
2:B:249:ARG:O	2:B:250:ARG:HG2	2.15	0.47
1:A:222:PHE:N	1:A:222:PHE:CD1	2.82	0.47
2:B:325:THR:OG1	2:B:445:VAL:HG11	2.15	0.47
2:B:352:ASN:C	2:B:352:ASN:ND2	2.67	0.47
2:B:205:LEU:CD1	2:B:611:VAL:HG11	2.44	0.47
2:B:699:ALA:HB1	2:B:921:LYS:HZ2	1.80	0.47
2:B:687:LYS:HZ2	2:B:925:SER:HA	1.80	0.46
2:B:388:ARG:HB2	2:B:389:PRO:HD2	1.97	0.46
1:A:702:LEU:CD2	1:A:709:PRO:HD2	2.45	0.46
1:A:485:ALA:HB2	1:A:511:LEU:CD1	2.39	0.46
1:A:362:THR:O	1:A:365:THR:O	2.32	0.46
2:B:224:GLU:HA	2:B:291:MET:HG3	1.96	0.46
2:B:314:GLN:CG	2:B:318:LYS:HE3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:PRO:HG2	2:B:708:ARG:HD3	1.97	0.46
1:A:440:GLY:O	1:A:442:THR:HG22	2.16	0.46
1:A:681:ASP:O	1:A:684:TYR:N	2.45	0.46
1:A:566:TYR:CD1	1:A:764:VAL:HG12	2.50	0.46
1:A:411:ASP:OD1	1:A:483:HIS:NE2	2.49	0.46
2:B:170:VAL:O	2:B:170:VAL:HG12	2.16	0.46
2:B:580:SER:O	2:B:581:ASP:HB2	2.14	0.46
2:B:600:VAL:HG13	2:B:604:ILE:HD11	1.96	0.46
1:A:180:ASN:HD22	1:A:180:ASN:N	2.14	0.46
1:A:594:GLN:HE21	1:A:594:GLN:HB3	1.65	0.46
2:B:230:ARG:HD2	2:B:235:ARG:O	2.15	0.46
2:B:761:ASP:O	2:B:762:MET:O	2.33	0.46
1:A:93:TYR:O	1:A:96:LEU:HG	2.15	0.46
2:B:795:GLU:O	2:B:797:TYR:N	2.49	0.46
1:A:197:LEU:HD13	1:A:227:PHE:CE1	2.51	0.46
1:A:725:LEU:HD23	1:A:728:LEU:HD12	1.98	0.46
2:B:352:ASN:C	2:B:352:ASN:HD22	2.11	0.46
1:A:564:ALA:HB2	1:A:576:LEU:HD13	1.98	0.46
1:A:756:MET:O	1:A:760:GLN:HG3	2.15	0.46
2:B:133:ARG:HG3	2:B:135:MET:HG2	1.97	0.45
2:B:378:ILE:HD13	2:B:385:PHE:CZ	2.51	0.45
1:A:629:LEU:HG	1:A:641:VAL:CG2	2.46	0.45
1:A:134:THR:HG22	1:A:138:ASP:OD2	2.16	0.45
2:B:144:LEU:HD22	2:B:918:GLN:NE2	2.31	0.45
1:A:450:LEU:H	1:A:450:LEU:HD12	1.80	0.45
2:B:292:ALA:HA	2:B:293:PRO:HD3	1.83	0.45
2:B:668:LEU:HD21	2:B:733:ARG:NH1	2.31	0.45
2:B:212:HIS:O	2:B:590:ARG:HB3	2.16	0.45
1:A:687:PHE:O	1:A:690:LEU:HB3	2.16	0.45
2:B:279:ASP:C	2:B:284:LYS:HE3	2.36	0.45
1:A:111:GLU:OE2	1:A:503:ARG:NH1	2.49	0.45
1:A:183:ARG:NH2	1:A:186:ARG:HD2	2.31	0.45
2:B:149:PRO:O	2:B:150:PRO:C	2.53	0.45
2:B:822:PHE:HD1	2:B:822:PHE:H	1.63	0.45
1:A:20:PRO:HG3	1:A:29:ASN:ND2	2.31	0.45
1:A:583:TYR:HB3	1:A:584:PRO:HD3	1.97	0.45
1:A:241:LEU:O	1:A:241:LEU:HD23	2.16	0.45
1:A:627:PRO:O	1:A:643:LEU:HD11	2.17	0.45
1:A:369:LEU:HD23	1:A:611:HIS:HB2	1.98	0.45
2:B:62:LEU:HA	2:B:66:GLN:OE1	2.17	0.45
1:A:92:GLN:N	1:A:92:GLN:OE1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:SER:O	2:B:317:ILE:HG12	2.16	0.45
2:B:417:ASN:HD21	2:B:419:ILE:HD12	1.81	0.45
1:A:236:PHE:HB3	4:A:820:HOH:O	2.16	0.45
2:B:756:VAL:O	2:B:786:PRO:HA	2.17	0.45
1:A:119:THR:O	1:A:120:VAL:O	2.34	0.44
1:A:550:ARG:CZ	1:A:550:ARG:HB2	2.47	0.44
2:B:750:LYS:HE3	2:B:805:GLY:CA	2.46	0.44
1:A:705:ARG:HD2	1:A:709:PRO:HD3	1.99	0.44
2:B:223:ASN:O	2:B:291:MET:HG2	2.17	0.44
2:B:424:LEU:O	2:B:428:LEU:HB2	2.17	0.44
2:B:900:SER:HA	2:B:907:ILE:HG21	1.97	0.44
1:A:238:LEU:HD23	1:A:238:LEU:O	2.17	0.44
2:B:300:GLN:O	2:B:301:PRO:C	2.56	0.44
2:B:672:ARG:NH1	2:B:725:SER:HA	2.32	0.44
2:B:419:ILE:HG22	2:B:421:ASN:H	1.82	0.44
2:B:309:LEU:C	2:B:309:LEU:HD12	2.38	0.44
2:B:571:PHE:HD2	2:B:596:PHE:CE1	2.35	0.44
2:B:908:LEU:C	2:B:910:ASN:H	2.21	0.44
2:B:668:LEU:O	2:B:671:ALA:HB3	2.18	0.44
2:B:253:CYS:SG	2:B:255:PHE:HB2	2.58	0.44
2:B:163:ILE:HD13	2:B:634:PRO:HG3	2.00	0.44
2:B:506:TYR:CE2	2:B:508:ASP:HB2	2.52	0.44
1:A:355:MET:O	1:A:359:LYS:HB2	2.17	0.44
2:B:147:LEU:O	2:B:149:PRO:N	2.50	0.44
1:A:598:VAL:HG23	1:A:598:VAL:O	2.17	0.44
2:B:150:PRO:O	2:B:151:ILE:HB	2.18	0.44
2:B:133:ARG:HH21	2:B:135:MET:HE2	1.83	0.44
2:B:68:GLN:O	2:B:72:GLN:HG3	2.17	0.44
1:A:359:LYS:HG2	1:A:363:ASP:OD2	2.18	0.43
1:A:234:VAL:HG13	1:A:234:VAL:O	2.18	0.43
2:B:920:MET:CA	2:B:920:MET:HE3	2.45	0.43
1:A:145:ILE:HA	1:A:148:LEU:HD12	2.00	0.43
1:A:182:PHE:CZ	1:A:197:LEU:HD21	2.51	0.43
2:B:242:VAL:CG1	2:B:251:TRP:HB2	2.48	0.43
1:A:119:THR:CG2	1:A:120:VAL:N	2.81	0.43
2:B:302:PRO:HA	2:B:303:PRO:HD3	1.73	0.43
1:A:567:ASN:O	1:A:568:LYS:C	2.57	0.43
2:B:729:PRO:HB2	2:B:732:HIS:CD2	2.52	0.43
1:A:55:VAL:HG12	1:A:56:CYS:N	2.33	0.43
2:B:919:ILE:HG22	2:B:923:ARG:HD2	1.99	0.43
1:A:587:THR:O	1:A:591:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASP:HA	1:A:141:LYS:HD3	2.01	0.43
2:B:791:SER:H	2:B:905:ASP:CG	2.21	0.43
1:A:382:GLN:HB3	1:A:708:LEU:HD11	1.99	0.43
2:B:147:LEU:HD23	2:B:147:LEU:HA	1.74	0.43
2:B:459:ARG:NH1	2:B:459:ARG:CG	2.79	0.43
1:A:674:ARG:C	1:A:676:ALA:H	2.22	0.43
2:B:224:GLU:HA	2:B:291:MET:CG	2.49	0.43
1:A:65:LEU:HD23	1:A:104:GLU:HG3	2.00	0.43
1:A:166:VAL:HG21	1:A:268:ILE:HG13	2.01	0.43
1:A:309:ARG:HD3	1:A:309:ARG:H	1.84	0.43
2:B:783:LEU:HA	2:B:784:PRO:HD3	1.81	0.43
1:A:564:ALA:HB2	1:A:576:LEU:CD1	2.49	0.43
2:B:168:MET:HG2	2:B:241:PHE:CE2	2.53	0.43
1:A:629:LEU:HD11	1:A:654:LEU:HB3	2.00	0.43
1:A:670:ILE:HD13	1:A:690:LEU:HD21	2.00	0.43
2:B:764:ASP:O	2:B:851:ARG:NH2	2.51	0.42
2:B:789:ALA:HB1	2:B:902:LEU:HA	2.01	0.42
1:A:20:PRO:HB3	1:A:25:ASP:CB	2.49	0.42
1:A:674:ARG:C	1:A:676:ALA:N	2.72	0.42
2:B:144:LEU:HD22	2:B:918:GLN:HE22	1.84	0.42
1:A:93:TYR:CE1	1:A:102:PRO:HB3	2.54	0.42
1:A:670:ILE:CD1	1:A:690:LEU:HD21	2.49	0.42
1:A:637:ASP:O	1:A:638:PRO:C	2.56	0.42
1:A:80:CYS:HA	1:A:81:PRO:HD3	1.86	0.42
2:B:361:LEU:HD23	2:B:399:CYS:SG	2.58	0.42
2:B:209:PRO:CG	2:B:558:MET:HE1	2.47	0.42
1:A:20:PRO:HG2	1:A:26:ALA:HA	2.00	0.42
1:A:708:LEU:N	1:A:708:LEU:HD23	2.33	0.42
2:B:497:VAL:HG12	2:B:499:LEU:HD11	2.01	0.42
1:A:665:TYR:C	1:A:665:TYR:CD2	2.92	0.42
2:B:802:ILE:HB	2:B:809:PHE:HB2	2.01	0.42
2:B:344:ARG:HA	2:B:394:VAL:O	2.18	0.42
2:B:250:ARG:HD2	2:B:260:ASN:O	2.18	0.42
1:A:39:PRO:O	1:A:503:ARG:HG2	2.20	0.42
1:A:191:GLU:O	1:A:195:GLU:HG3	2.19	0.42
2:B:864:ASP:N	2:B:864:ASP:OD1	2.53	0.42
2:B:253:CYS:O	2:B:257:ARG:HA	2.19	0.42
1:A:20:PRO:HB3	1:A:25:ASP:HB3	2.02	0.42
1:A:386:ARG:NH1	1:A:705:ARG:O	2.49	0.42
2:B:359:ILE:HD11	2:B:406:LEU:HD23	2.01	0.42
1:A:625:ILE:O	1:A:627:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:VAL:CG1	2:B:243:THR:N	2.83	0.42
1:A:663:LEU:HD23	1:A:663:LEU:C	2.40	0.42
2:B:151:ILE:HD13	2:B:709:MET:CE	2.50	0.42
1:A:671:ALA:O	1:A:675:LYS:N	2.42	0.42
2:B:138:LEU:HB2	4:B:953:HOH:O	2.20	0.42
1:A:129:ASP:HB2	1:A:162:TYR:CZ	2.55	0.42
2:B:546:LYS:NZ	2:B:862:HIS:O	2.52	0.42
2:B:209:PRO:CG	2:B:558:MET:CE	2.97	0.42
1:A:130:LEU:HD11	1:A:161:THR:HB	2.00	0.42
2:B:151:ILE:HD13	2:B:709:MET:HE1	2.02	0.42
1:A:669:GLN:NE2	1:A:669:GLN:CA	2.74	0.42
2:B:333:LEU:HD12	2:B:400:ARG:NE	2.35	0.42
1:A:447:MET:N	1:A:447:MET:SD	2.93	0.42
2:B:553:CYS:O	2:B:587:THR:HA	2.19	0.41
1:A:587:THR:HG22	1:A:591:ARG:HD2	2.02	0.41
1:A:130:LEU:CD1	1:A:161:THR:HB	2.50	0.41
1:A:49:ALA:HB1	1:A:51:TYR:CZ	2.55	0.41
1:A:66:ASN:HB2	1:A:67:PRO:CD	2.50	0.41
1:A:124:PHE:CE1	1:A:151:LEU:HD22	2.55	0.41
2:B:212:HIS:CD2	2:B:217:ILE:HB	2.55	0.41
1:A:750:VAL:HG12	1:A:751:SER:N	2.27	0.41
2:B:187:ASN:O	2:B:634:PRO:HD2	2.20	0.41
2:B:717:LEU:HD12	2:B:717:LEU:HA	1.83	0.41
1:A:238:LEU:HD23	1:A:238:LEU:C	2.41	0.41
1:A:642:LEU:O	1:A:644:ASP:N	2.47	0.41
1:A:89:LEU:HD12	1:A:90:PRO:HD2	2.03	0.41
2:B:362:ASP:CG	2:B:401:GLN:HB2	2.41	0.41
1:A:609:TYR:HA	1:A:660:PHE:CE2	2.54	0.41
2:B:781:ILE:HB	2:B:858:GLN:OE1	2.21	0.41
1:A:349:CYS:HA	1:A:373:ASP:O	2.21	0.41
1:A:21:SER:HA	1:A:511:LEU:HD23	2.02	0.41
2:B:277:ARG:C	2:B:279:ASP:N	2.74	0.41
2:B:820:LEU:C	2:B:822:PHE:N	2.74	0.41
1:A:594:GLN:OE1	1:A:727:LYS:NZ	2.49	0.41
1:A:658:THR:O	1:A:659:PHE:HB3	2.21	0.41
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.89	0.41
2:B:279:ASP:HA	2:B:284:LYS:CE	2.48	0.41
2:B:799:LEU:HD13	2:B:812:MET:CE	2.50	0.41
2:B:799:LEU:HD13	2:B:812:MET:HE3	2.02	0.41
2:B:496:THR:OG1	2:B:587:THR:HG23	2.20	0.41
1:A:93:TYR:CD1	1:A:102:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:ASP:CB	2:B:273:ASP:HB3	2.50	0.41
1:A:574:PHE:CD2	1:A:760:GLN:HG2	2.56	0.41
1:A:639:GLN:HA	1:A:640:PRO:HD3	1.81	0.41
2:B:560:ALA:HA	2:B:612:GLN:O	2.21	0.41
1:A:369:LEU:HB3	1:A:611:HIS:CD2	2.56	0.41
2:B:242:VAL:HG12	2:B:243:THR:N	2.34	0.41
2:B:163:ILE:HA	2:B:164:PRO:HD3	1.90	0.40
1:A:282:ALA:HB3	1:A:341:HIS:CD2	2.56	0.40
2:B:633:MET:HA	2:B:634:PRO:HD3	1.89	0.40
1:A:591:ARG:HG3	1:A:591:ARG:NH1	2.35	0.40
1:A:123:ILE:HG12	1:A:156:LEU:HB2	2.02	0.40
2:B:301:PRO:HA	2:B:302:PRO:HD3	1.68	0.40
1:A:309:ARG:N	1:A:309:ARG:HD3	2.36	0.40
2:B:336:ILE:HA	2:B:337:PRO:HD3	1.91	0.40
2:B:441:LYS:HD2	2:B:552:PHE:CE2	2.57	0.40
2:B:329:LEU:O	2:B:333:LEU:HD23	2.22	0.40
1:A:453:TYR:CE2	1:A:704:ASP:O	2.75	0.40
2:B:872:TYR:CE2	2:B:897:TRP:CZ3	3.06	0.40
1:A:594:GLN:OE1	1:A:658:THR:HG21	2.21	0.40
2:B:217:ILE:C	2:B:219:PRO:HD3	2.41	0.40
1:A:181:VAL:HB	2:B:378:ILE:HG12	2.04	0.40
2:B:623:GLN:OE1	2:B:625:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/768 (90%)	631 (91%)	52 (8%)	12 (2%)	11	32
2	B	734/926 (79%)	651 (89%)	55 (8%)	28 (4%)	4	11
All	All	1429/1694 (84%)	1282 (90%)	107 (8%)	40 (3%)	6	18

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	120	VAL
1	A	234	VAL
1	A	254	ALA
1	A	678	TYR
2	B	147	LEU
2	B	148	PRO
2	B	151	ILE
2	B	601	ASP
2	B	762	MET
2	B	766	ALA
2	B	767	GLY
2	B	796	ARG
1	A	409	SER
1	A	643	LEU
1	A	675	LYS
2	B	278	TYR
2	B	313	SER
2	B	415	GLN
2	B	469	SER
2	B	580	SER
2	B	697	GLY
2	B	867	THR
2	B	903	VAL
2	B	479	GLN
2	B	530	SER
2	B	620	ASN
2	B	724	ARG
2	B	793	LEU
1	A	751	SER
2	B	149	PRO
1	A	94	THR
2	B	818	PRO
2	B	859	LEU
2	B	146	GLU
2	B	215	ASP
2	B	271	PRO
2	B	763	ALA
1	A	82	ILE
1	A	598	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	621/668 (93%)	595 (96%)	26 (4%)	36	68
2	B	672/819 (82%)	652 (97%)	20 (3%)	48	80
All	All	1293/1487 (87%)	1247 (96%)	46 (4%)	42	75

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	83	CYS
1	A	125	PHE
1	A	164	ASN
1	A	174	GLU
1	A	222	PHE
1	A	234	VAL
1	A	239	ASN
1	A	298	LEU
1	A	309	ARG
1	A	436	GLU
1	A	447	MET
1	A	450	LEU
1	A	499	THR
1	A	503	ARG
1	A	534	ARG
1	A	552	LEU
1	A	576	LEU
1	A	591	ARG
1	A	594	GLN
1	A	647	SER
1	A	651	ASN
1	A	669	GLN
1	A	674	ARG
1	A	682	PRO
1	A	683	GLN
2	B	138	LEU

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Mol	Chain	Res	Type
2	B	150	PRO
2	B	152	THR
2	B	166	GLU
2	B	208	ARG
2	B	213	LEU
2	B	309	LEU
2	B	352	ASN
2	B	377	ASP
2	B	428	LEU
2	B	459	ARG
2	B	557	VAL
2	B	618	SER
2	B	739	ASN
2	B	743	LEU
2	B	751	ASN
2	B	761	ASP
2	B	764	ASP
2	B	822	PHE
2	B	870	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	244	ASN
1	A	256	HIS
1	A	301	ASN
1	A	318	HIS
1	A	339	ASN
1	A	382	GLN
1	A	585	GLN
1	A	620	ASN
1	A	651	ASN
1	A	669	GLN
1	A	760	GLN
2	B	72	GLN
2	B	352	ASN
2	B	372	GLN
2	B	374	ASN
2	B	421	ASN
2	B	479	GLN
2	B	485	ASN

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Mol	Chain	Res	Type
2	B	533	ASN
2	B	535	ASN
2	B	599	ASN
2	B	732	HIS
2	B	857	ASN
2	B	918	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 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 ⓘ

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.