



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:18 pm BST

PDB ID : 1XDV  
Title : Experimentally Phased Structure of Human the Son of Sevenless protein at 4.1 Å.  
Authors : Sondermann, H.; Soisson, S.M.; Boykevisch, S.; Yang, S.S.; Bar-Sagi, D.; Kuriyan, J.  
Deposited on : 2004-09-08  
Resolution : 4.10 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

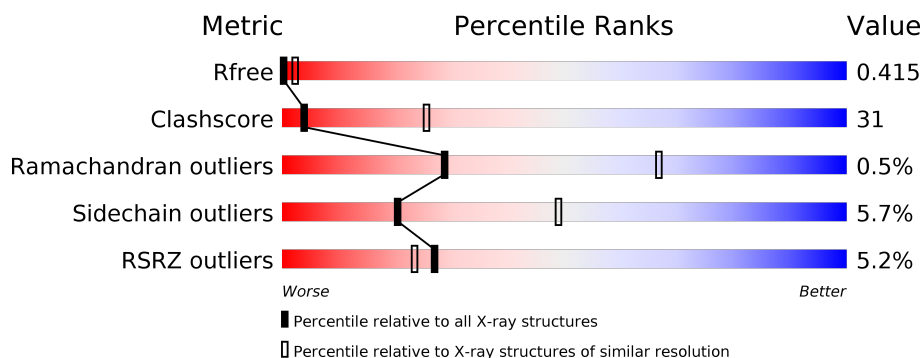
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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))
$R_{free}$	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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 respectively. 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	847	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	847	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>29%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12516 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.

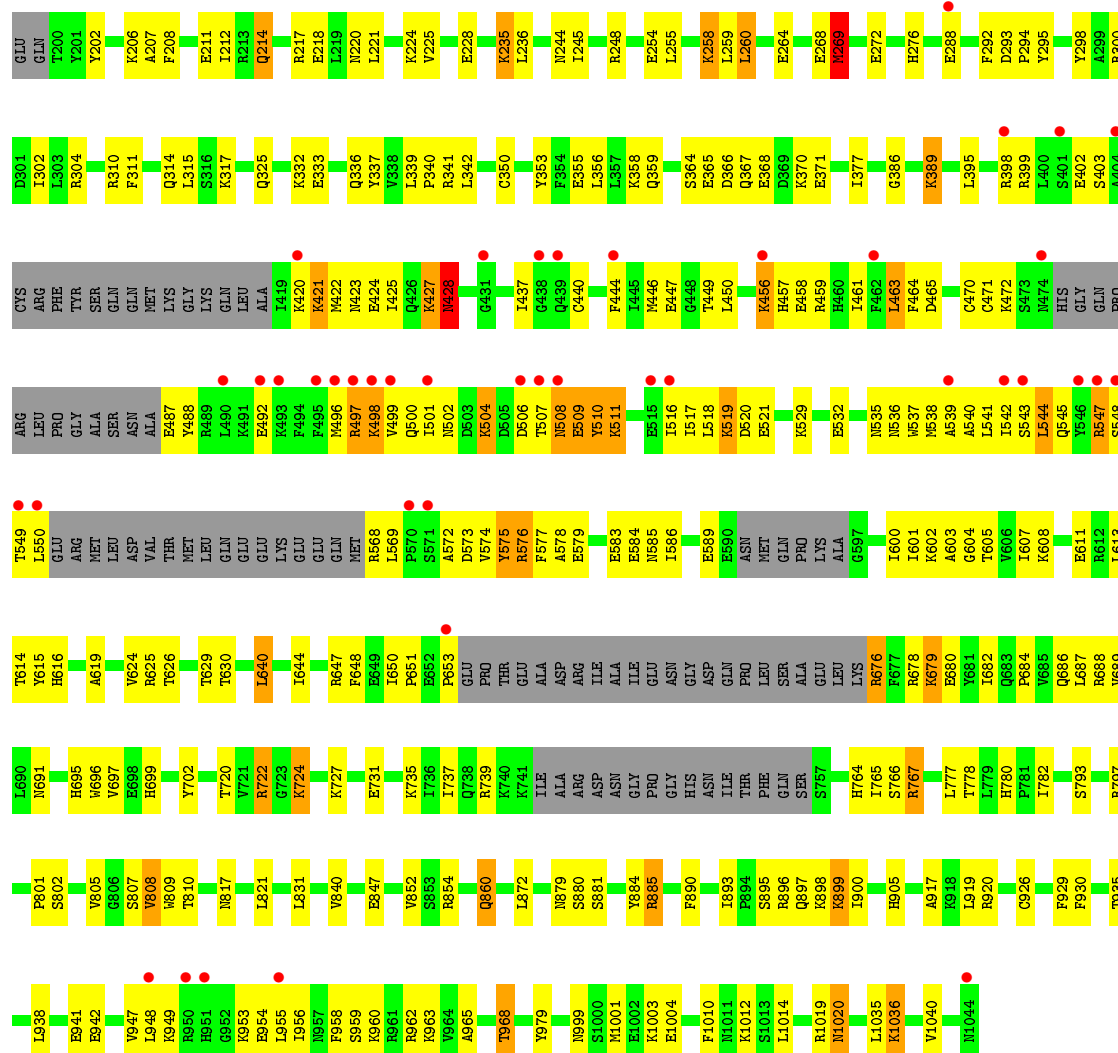
- Molecule 1 is a protein called Son of sevenless protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	0	0
			6254	4009	1066	1151	28			
1	B	759	Total	C	N	O	S	0	0	0
			6262	4015	1067	1152	28			



- Molecule 1: Son of sevenless protein homolog 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.03Å 124.71Å 245.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.10 49.19 – 4.10	Depositor EDS
% Data completeness (in resolution range)	91.0 (8.00-4.10) 94.5 (49.19-4.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 4.14Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.433 , 0.449 0.403 , 0.415	Depositor DCC
$R_{free}$ test set	1858 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	12516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 [i](#)

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

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	0.39	2/6390 (0.0%)	0.61	2/8615 (0.0%)
1	B	0.40	3/6398 (0.0%)	0.61	2/8626 (0.0%)
All	All	0.39	5/12788 (0.0%)	0.61	4/17241 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	MET	CG-SD	6.62	1.98	1.81
1	B	427	LYS	CA-C	-5.53	1.38	1.52
1	A	427	LYS	CA-C	-5.50	1.38	1.52
1	A	428	ASN	N-CA	-5.18	1.35	1.46
1	B	428	ASN	N-CA	-5.18	1.35	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	MET	CG-SD-CE	7.27	111.83	100.20
1	B	1020	ASN	N-CA-C	5.13	124.86	111.00
1	A	1020	ASN	N-CA-C	5.13	124.84	111.00
1	A	304	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	6254	0	6262	384	122
1	B	6262	0	6267	477	116
All	All	12516	0	12529	766	122

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 31.

All (766) 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:269:MET:CE	1:A:729:TRP:CZ2	1.75	1.68
1:A:1019:ARG:HH22	1:B:905:HIS:CE1	1.17	1.60
1:B:342:LEU:HD21	1:B:550:LEU:CD1	1.20	1.58
1:B:269:MET:CG	1:B:691:ASN:HD21	0.94	1.58
1:A:269:MET:HE2	1:A:729:TRP:CZ2	1.25	1.56
1:A:630:THR:HG22	1:A:969:GLY:CA	1.24	1.56
1:A:630:THR:CG2	1:A:969:GLY:HA3	1.26	1.54
1:B:602:LYS:HE2	1:B:948:LEU:CD1	1.36	1.51
1:B:268:GLU:CD	1:B:619:ALA:CB	1.78	1.48
1:A:905:HIS:CD2	1:B:1019:ARG:HH12	1.32	1.48
1:B:342:LEU:CD2	1:B:550:LEU:HD13	1.43	1.46
1:B:402:GLU:CG	1:B:536:ASN:HA	1.45	1.46
1:A:905:HIS:CE1	1:B:1019:ARG:HH22	1.32	1.44
1:A:304:ARG:NH2	1:A:399:ARG:NH1	1.63	1.44
1:B:342:LEU:CD2	1:B:550:LEU:CD1	1.97	1.43
1:A:1019:ARG:HH12	1:B:905:HIS:CD2	1.37	1.42
1:B:402:GLU:OE2	1:B:536:ASN:N	1.58	1.35
1:A:269:MET:CE	1:A:729:TRP:CE2	2.12	1.33
1:A:1019:ARG:NH2	1:B:905:HIS:CE1	1.96	1.29
1:B:268:GLU:OE2	1:B:619:ALA:CB	1.78	1.29
1:B:398:ARG:HG2	1:B:532:GLU:OE2	1.13	1.29
1:B:337:TYR:CB	1:B:538:MET:HE2	1.64	1.26
1:A:269:MET:CG	1:A:691:ASN:HD21	1.48	1.26
1:A:269:MET:HG2	1:A:691:ASN:ND2	1.52	1.25
1:B:630:THR:CA	1:B:805:VAL:HG11	1.66	1.24
1:B:217:ARG:NE	1:B:548:SER:O	1.68	1.24
1:A:905:HIS:CD2	1:B:1019:ARG:NH1	2.08	1.22
1:A:269:MET:HE2	1:A:729:TRP:CE2	1.71	1.21
1:A:304:ARG:NE	1:A:307:PHE:HB2	1.54	1.21
1:A:1019:ARG:NH1	1:B:905:HIS:CD2	2.07	1.21
1:A:935:THR:OG1	1:B:1004:GLU:OE2	1.60	1.20
1:A:905:HIS:CE1	1:B:1019:ARG:NH2	2.10	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:GLU:OE1	1:B:999:ASN:ND2	1.77	1.18
1:B:342:LEU:HD22	1:B:550:LEU:CD2	1.73	1.17
1:A:304:ARG:CD	1:A:307:PHE:HB2	1.75	1.16
1:B:584:GLU:HG2	1:B:953:LYS:CD	1.76	1.16
1:B:269:MET:HG2	1:B:691:ASN:ND2	1.41	1.14
1:A:634:PHE:HB2	1:A:958:PHE:CZ	1.83	1.13
1:A:304:ARG:CZ	1:A:307:PHE:HB2	1.78	1.13
1:B:342:LEU:HD22	1:B:550:LEU:HD22	1.14	1.13
1:B:268:GLU:OE2	1:B:619:ALA:HB1	0.95	1.13
1:B:342:LEU:HD13	1:B:550:LEU:HD21	1.26	1.12
1:B:402:GLU:HG2	1:B:536:ASN:HA	1.30	1.12
1:B:584:GLU:HG2	1:B:953:LYS:HD2	1.16	1.12
1:B:604:GLY:H	1:B:956:ILE:HB	1.01	1.11
1:A:884:TYR:CE2	1:B:885:ARG:HB3	1.85	1.11
1:B:402:GLU:CG	1:B:536:ASN:CA	2.14	1.10
1:A:629:THR:CG2	1:A:969:GLY:O	2.00	1.09
1:B:602:LYS:CE	1:B:948:LEU:HD11	1.83	1.09
1:B:341:ARG:HG2	1:B:539:ALA:CA	1.48	1.09
1:B:630:THR:HA	1:B:805:VAL:HG11	1.09	1.09
1:B:337:TYR:HB3	1:B:538:MET:HE2	1.10	1.08
1:B:341:ARG:CG	1:B:539:ALA:HA	1.81	1.07
1:B:602:LYS:CE	1:B:948:LEU:CD1	2.31	1.07
1:A:506:ASP:OD1	1:A:508:ASN:HB3	1.54	1.07
1:B:218:GLU:HG2	1:B:550:LEU:HA	1.32	1.07
1:B:268:GLU:CD	1:B:619:ALA:HB1	1.57	1.07
1:A:269:MET:HE3	1:A:729:TRP:CZ2	1.62	1.07
1:A:885:ARG:HB3	1:B:884:TYR:CE2	1.89	1.06
1:B:341:ARG:HG2	1:B:539:ALA:HA	1.34	1.06
1:B:604:GLY:N	1:B:956:ILE:HB	1.71	1.06
1:B:506:ASP:OD2	1:B:508:ASN:HB3	1.56	1.05
1:B:268:GLU:CD	1:B:619:ALA:HB3	1.72	1.04
1:B:602:LYS:HE2	1:B:948:LEU:HD12	1.31	1.04
1:B:217:ARG:CZ	1:B:548:SER:O	2.05	1.04
1:B:398:ARG:CG	1:B:532:GLU:OE2	2.06	1.04
1:A:304:ARG:CZ	1:A:307:PHE:CB	2.36	1.04
1:A:269:MET:HE3	1:A:729:TRP:CH2	1.92	1.04
1:A:938:LEU:HD21	1:B:999:ASN:HB2	1.41	1.03
1:A:905:HIS:ND1	1:B:1019:ARG:NH2	2.06	1.03
1:B:337:TYR:CG	1:B:538:MET:HE2	1.94	1.03
1:B:342:LEU:HD21	1:B:550:LEU:HD11	1.05	1.02
1:B:342:LEU:CD1	1:B:550:LEU:HD21	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:VAL:HG23	1:A:517:ILE:HB	1.39	1.02
1:B:217:ARG:NH2	1:B:548:SER:O	1.92	1.02
1:A:303:LEU:HA	1:A:304:ARG:HH21	1.24	1.01
1:A:905:HIS:CE1	1:B:1014:LEU:HD11	1.93	1.01
1:B:767:ARG:HH11	1:B:767:ARG:H	1.02	1.00
1:A:885:ARG:HB3	1:B:884:TYR:HE2	1.20	1.00
1:A:884:TYR:HE2	1:B:885:ARG:HB3	1.16	1.00
1:A:935:THR:HG1	1:B:1004:GLU:CD	1.65	1.00
1:B:269:MET:CB	1:B:691:ASN:HD21	1.74	1.00
1:B:584:GLU:CG	1:B:953:LYS:HD2	1.91	1.00
1:B:217:ARG:HH21	1:B:548:SER:C	1.65	1.00
1:B:602:LYS:HE2	1:B:948:LEU:HD11	1.04	0.99
1:B:341:ARG:CG	1:B:539:ALA:CA	2.17	0.97
1:B:337:TYR:CG	1:B:538:MET:CE	2.47	0.97
1:B:337:TYR:CB	1:B:538:MET:CE	2.43	0.97
1:B:422:MET:HE3	1:B:437:ILE:HG22	1.46	0.97
1:A:1004:GLU:OE2	1:B:935:THR:OG1	1.82	0.97
1:A:1019:ARG:NH2	1:B:905:HIS:ND1	2.03	0.96
1:B:604:GLY:H	1:B:956:ILE:CB	1.78	0.96
1:A:634:PHE:HB2	1:A:958:PHE:HZ	1.22	0.96
1:B:601:ILE:O	1:B:958:PHE:HB3	1.67	0.94
1:A:630:THR:HB	1:A:965:ALA:O	1.68	0.94
1:B:583:GLU:O	1:B:955:LEU:HD21	1.68	0.94
1:A:304:ARG:HH11	1:A:307:PHE:H	0.94	0.94
1:B:269:MET:HB3	1:B:691:ASN:OD1	1.64	0.94
1:A:337:TYR:OH	1:A:502:ASN:ND2	2.01	0.94
1:B:269:MET:HG2	1:B:691:ASN:HD21	0.77	0.93
1:A:999:ASN:ND2	1:B:942:GLU:OE1	1.99	0.93
1:B:342:LEU:CD2	1:B:550:LEU:CD2	2.47	0.93
1:A:269:MET:SD	1:A:687:LEU:HD11	2.09	0.93
1:A:269:MET:HG2	1:A:691:ASN:HD21	0.78	0.93
1:B:268:GLU:CD	1:B:619:ALA:HB2	1.88	0.93
1:B:499:VAL:HG12	1:B:517:ILE:HB	1.51	0.93
1:B:269:MET:CG	1:B:691:ASN:ND2	1.78	0.92
1:A:422:MET:HE3	1:A:437:ILE:HG22	1.50	0.92
1:A:1004:GLU:CD	1:B:935:THR:HG1	1.71	0.92
1:A:905:HIS:CG	1:B:1019:ARG:HH22	1.88	0.92
1:A:302:ILE:O	1:A:304:ARG:NH2	2.02	0.92
1:B:630:THR:HA	1:B:805:VAL:CG1	1.99	0.92
1:A:304:ARG:NH1	1:A:307:PHE:CB	2.31	0.91
1:A:301:ASP:O	1:A:304:ARG:HG3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:THR:HG22	1:A:969:GLY:O	1.68	0.91
1:B:268:GLU:CG	1:B:619:ALA:HB2	1.99	0.91
1:B:342:LEU:HD21	1:B:550:LEU:HD13	0.99	0.91
1:B:496:MET:HA	1:B:498:LYS:HZ3	1.34	0.91
1:B:358:LYS:HE3	1:B:377:ILE:HD13	1.53	0.90
1:B:218:GLU:HG2	1:B:550:LEU:CA	2.01	0.90
1:B:630:THR:CB	1:B:805:VAL:HG11	2.03	0.89
1:A:304:ARG:NH1	1:A:307:PHE:HB3	1.88	0.88
1:B:337:TYR:HB3	1:B:538:MET:CE	2.00	0.88
1:A:304:ARG:HH11	1:A:307:PHE:N	1.71	0.88
1:A:935:THR:OG1	1:B:1004:GLU:CD	2.11	0.87
1:A:614:THR:HG23	1:A:688:ARG:HB2	1.56	0.87
1:B:268:GLU:OE1	1:B:619:ALA:HB3	1.72	0.87
1:A:1019:ARG:HH22	1:B:905:HIS:CG	1.92	0.87
1:A:881:SER:N	1:B:881:SER:OG	2.08	0.87
1:B:402:GLU:CD	1:B:536:ASN:N	2.29	0.86
1:A:269:MET:CE	1:A:687:LEU:HD11	2.05	0.85
1:B:614:THR:HG23	1:B:688:ARG:HB2	1.56	0.85
1:A:303:LEU:HA	1:A:304:ARG:NH2	1.90	0.85
1:A:629:THR:HG22	1:A:969:GLY:C	1.95	0.85
1:B:269:MET:CB	1:B:691:ASN:ND2	2.34	0.85
1:A:905:HIS:NE2	1:B:1014:LEU:CD1	2.40	0.85
1:A:881:SER:OG	1:B:881:SER:N	2.10	0.85
1:B:398:ARG:HG2	1:B:532:GLU:CD	1.97	0.85
1:A:1014:LEU:HD11	1:B:905:HIS:CE1	2.12	0.85
1:B:402:GLU:CD	1:B:536:ASN:CA	2.45	0.84
1:A:896:ARG:O	1:A:899:LYS:HG2	1.78	0.84
1:B:268:GLU:CG	1:B:619:ALA:CB	2.56	0.83
1:B:402:GLU:CD	1:B:536:ASN:HA	1.98	0.83
1:A:303:LEU:CA	1:A:304:ARG:HH21	1.91	0.83
1:A:1019:ARG:NH1	1:B:905:HIS:NE2	2.18	0.83
1:A:269:MET:HE2	1:A:729:TRP:HZ2	1.03	0.82
1:A:1019:ARG:NH2	1:B:905:HIS:CG	2.47	0.82
1:A:630:THR:HG22	1:A:969:GLY:N	1.93	0.82
1:A:905:HIS:CG	1:B:1019:ARG:NH2	2.47	0.82
1:A:304:ARG:NE	1:A:304:ARG:N	2.28	0.82
1:B:202:TYR:O	1:B:206:LYS:HG3	1.80	0.81
1:B:499:VAL:CG1	1:B:517:ILE:HB	2.10	0.81
1:B:341:ARG:CZ	1:B:539:ALA:H	1.94	0.81
1:B:366:ASP:OD2	1:B:368:GLU:HG2	1.79	0.81
1:B:767:ARG:HH11	1:B:767:ARG:N	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:NH1	1:A:307:PHE:H	1.78	0.80
1:A:202:TYR:O	1:A:206:LYS:HG3	1.81	0.80
1:B:506:ASP:OD2	1:B:508:ASN:CB	2.29	0.79
1:A:938:LEU:HD21	1:B:999:ASN:CB	2.13	0.79
1:B:220:ASN:HB3	1:B:224:LYS:NZ	1.98	0.78
1:B:584:GLU:HG2	1:B:953:LYS:CG	2.14	0.78
1:B:498:LYS:HG3	1:B:518:LEU:HD13	1.63	0.78
1:A:269:MET:HE3	1:A:687:LEU:HD11	1.66	0.78
1:A:929:PHE:CE1	1:B:1003:LYS:HE3	2.19	0.78
1:A:304:ARG:CZ	1:A:307:PHE:HB3	2.12	0.78
1:A:905:HIS:NE2	1:B:1014:LEU:HD13	1.98	0.78
1:A:629:THR:OG1	1:A:973:GLN:OE1	2.00	0.77
1:A:341:ARG:NH2	1:A:536:ASN:OD1	2.17	0.77
1:A:519:LYS:HD3	1:A:519:LYS:H	1.50	0.77
1:B:268:GLU:HG2	1:B:619:ALA:HB2	1.65	0.77
1:B:496:MET:HA	1:B:498:LYS:NZ	1.99	0.77
1:B:342:LEU:CD2	1:B:550:LEU:HD22	2.06	0.77
1:A:1019:ARG:CZ	1:B:905:HIS:CD2	2.67	0.76
1:B:630:THR:HG22	1:B:805:VAL:CG2	2.15	0.76
1:A:1001:MET:HE3	1:B:810:THR:HG22	1.67	0.76
1:A:697:VAL:HG11	1:A:737:ILE:HG12	1.67	0.76
1:B:498:LYS:HE2	1:B:498:LYS:O	1.84	0.76
1:A:999:ASN:HB2	1:B:938:LEU:HD21	1.67	0.76
1:B:342:LEU:HD22	1:B:550:LEU:HD13	1.65	0.76
1:B:767:ARG:H	1:B:767:ARG:NH1	1.82	0.76
1:A:304:ARG:CD	1:A:307:PHE:CB	2.63	0.76
1:A:634:PHE:CB	1:A:958:PHE:CZ	2.68	0.76
1:B:341:ARG:HG2	1:B:539:ALA:C	2.06	0.76
1:A:1019:ARG:NH2	1:B:905:HIS:NE2	2.34	0.76
1:B:601:ILE:O	1:B:958:PHE:CD2	2.38	0.75
1:A:544:LEU:HA	1:A:547:ARG:HH12	1.50	0.75
1:B:697:VAL:HG11	1:B:737:ILE:HG12	1.67	0.75
1:A:1004:GLU:CD	1:B:935:THR:OG1	2.21	0.75
1:A:258:LYS:HE2	1:A:286:LEU:HD21	1.68	0.75
1:B:498:LYS:HG3	1:B:518:LEU:HA	1.69	0.74
1:B:342:LEU:HD13	1:B:550:LEU:CD2	2.11	0.74
1:A:1003:LYS:HE3	1:B:929:PHE:CE1	2.21	0.74
1:B:342:LEU:CD2	1:B:550:LEU:CG	2.66	0.74
1:B:402:GLU:OE2	1:B:536:ASN:CA	2.34	0.74
1:B:402:GLU:OE2	1:B:535:ASN:C	2.26	0.74
1:B:584:GLU:CG	1:B:953:LYS:CD	2.57	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:GLU:O	1:B:955:LEU:CD2	2.35	0.74
1:A:341:ARG:HH12	1:A:535:ASN:HB3	1.52	0.74
1:A:884:TYR:OH	1:B:885:ARG:HD2	1.87	0.73
1:B:342:LEU:HD22	1:B:550:LEU:CG	2.18	0.73
1:A:269:MET:HE1	1:A:729:TRP:CE2	2.19	0.73
1:A:314:GLN:NE2	1:A:317:LYS:HZ3	1.87	0.73
1:B:446:MET:HE1	1:B:537:TRP:HA	1.70	0.73
1:A:422:MET:CE	1:A:437:ILE:HG22	2.20	0.72
1:A:634:PHE:CB	1:A:958:PHE:HZ	2.01	0.72
1:A:905:HIS:NE2	1:B:1019:ARG:NH1	2.27	0.72
1:B:508:ASN:O	1:B:509:GLU:HG3	1.90	0.72
1:A:905:HIS:NE2	1:B:1014:LEU:HD11	2.04	0.72
1:A:1019:ARG:HH22	1:B:905:HIS:ND1	1.29	0.71
1:A:269:MET:O	1:A:694:ARG:NH1	2.23	0.71
1:B:244:ASN:HB3	1:B:310:ARG:NH2	2.06	0.71
1:B:300:ARG:O	1:B:304:ARG:HG3	1.90	0.71
1:B:207:ALA:O	1:B:211:GLU:HG3	1.91	0.71
1:B:221:LEU:HD13	1:B:549:THR:OG1	1.90	0.70
1:A:265:ASP:HB3	1:A:687:LEU:HD21	1.72	0.70
1:B:702:TYR:CE1	1:B:802:SER:OG	2.14	0.70
1:A:207:ALA:O	1:A:211:GLU:HG3	1.91	0.70
1:B:342:LEU:HD22	1:B:550:LEU:CD1	2.09	0.70
1:A:446:MET:HE1	1:A:537:TRP:HA	1.74	0.70
1:B:422:MET:CE	1:B:437:ILE:HG22	2.20	0.70
1:A:942:GLU:CD	1:B:999:ASN:ND2	2.44	0.70
1:A:879:ASN:HB3	1:B:1010:PHE:CZ	2.27	0.70
1:B:314:GLN:NE2	1:B:317:LYS:HZ3	1.90	0.70
1:A:905:HIS:CD2	1:B:1019:ARG:CZ	2.74	0.69
1:A:880:SER:C	1:B:881:SER:HG	1.95	0.69
1:B:421:LYS:HA	1:B:421:LYS:HE2	1.73	0.69
1:B:220:ASN:HB3	1:B:224:LYS:HZ1	1.56	0.69
1:A:604:GLY:O	1:A:962:ARG:NH2	2.26	0.69
1:A:304:ARG:HD3	1:A:307:PHE:HB2	1.69	0.69
1:A:355:GLU:HG3	1:A:359:GLN:HE21	1.58	0.69
1:A:500:GLN:OE1	1:A:516:ILE:HG12	1.93	0.69
1:B:629:THR:HG22	1:B:805:VAL:HG21	1.74	0.69
1:A:679:LYS:HD2	1:A:679:LYS:O	1.93	0.69
1:A:498:LYS:HG2	1:A:518:LEU:HA	1.75	0.68
1:B:947:VAL:HG11	1:B:954:GLU:HG3	1.76	0.68
1:A:498:LYS:HG2	1:A:518:LEU:HD23	1.75	0.68
1:B:355:GLU:HG3	1:B:359:GLN:HE21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ARG:HH22	1:B:905:HIS:CD2	2.11	0.68
1:A:446:MET:HE3	1:A:537:TRP:CE3	2.29	0.68
1:B:342:LEU:HD23	1:B:550:LEU:HD13	1.66	0.68
1:B:629:THR:HG23	1:B:801:PRO:HB2	1.76	0.68
1:B:601:ILE:O	1:B:958:PHE:CB	2.41	0.68
1:B:602:LYS:HA	1:B:958:PHE:HB3	1.76	0.68
1:B:218:GLU:HG2	1:B:550:LEU:C	2.15	0.67
1:A:506:ASP:CG	1:A:508:ASN:HB3	2.13	0.67
1:B:337:TYR:CG	1:B:538:MET:HE1	2.29	0.67
1:B:679:LYS:HD2	1:B:679:LYS:O	1.93	0.67
1:A:634:PHE:HB2	1:A:958:PHE:CE2	2.28	0.67
1:B:341:ARG:CZ	1:B:539:ALA:N	2.54	0.67
1:A:276:HIS:HE1	1:A:365:GLU:H	1.42	0.67
1:B:547:ARG:NH1	1:B:547:ARG:HB3	2.09	0.67
1:A:840:VAL:HG13	1:A:1012:LYS:HB3	1.76	0.67
1:B:220:ASN:O	1:B:224:LYS:HG2	1.95	0.67
1:A:1019:ARG:NH2	1:B:905:HIS:CD2	2.62	0.67
1:A:341:ARG:HG3	1:A:403:SER:OG	1.95	0.67
1:A:929:PHE:HE1	1:B:1003:LYS:HE3	1.59	0.67
1:A:609:LEU:CD2	1:A:962:ARG:NH1	2.58	0.66
1:A:529:LYS:HE3	1:A:533:GLU:OE2	1.95	0.66
1:A:630:THR:HG23	1:A:969:GLY:HA3	1.62	0.66
1:B:840:VAL:HG13	1:B:1012:LYS:HB3	1.76	0.66
1:B:276:HIS:HE1	1:B:365:GLU:H	1.42	0.66
1:A:1003:LYS:CE	1:B:929:PHE:HE1	2.08	0.66
1:B:341:ARG:HG3	1:B:403:SER:OG	1.95	0.66
1:A:947:VAL:HG11	1:A:954:GLU:HG3	1.76	0.66
1:B:602:LYS:CA	1:B:958:PHE:HB3	2.25	0.66
1:A:881:SER:HG	1:B:880:SER:C	1.98	0.66
1:A:1019:ARG:CZ	1:B:905:HIS:NE2	2.59	0.66
1:A:1014:LEU:CD1	1:B:905:HIS:NE2	2.59	0.65
1:A:506:ASP:OD1	1:A:508:ASN:CB	2.38	0.65
1:A:1003:LYS:HE3	1:B:929:PHE:CZ	2.30	0.65
1:B:614:THR:HG21	1:B:689:VAL:HG23	1.78	0.65
1:A:880:SER:C	1:B:881:SER:OG	2.34	0.65
1:B:314:GLN:NE2	1:B:317:LYS:NZ	2.44	0.65
1:A:885:ARG:HD2	1:B:884:TYR:OH	1.96	0.65
1:A:614:THR:HG21	1:A:689:VAL:HG23	1.77	0.65
1:A:314:GLN:NE2	1:A:317:LYS:NZ	2.44	0.65
1:A:544:LEU:HA	1:A:547:ARG:NH1	2.11	0.65
1:A:547:ARG:HH11	1:A:547:ARG:HB2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:PHE:HE1	1:B:1003:LYS:CE	2.10	0.65
1:B:793:SER:O	1:B:797:ARG:HG3	1.97	0.65
1:B:336:GLN:NE2	1:B:502:ASN:ND2	2.45	0.65
1:B:500:GLN:NE2	1:B:545:GLN:HB2	2.12	0.65
1:A:810:THR:HG22	1:B:1001:MET:HE3	1.77	0.64
1:B:589:GLU:OE1	1:B:959:SER:HB2	1.97	0.64
1:A:507:THR:C	1:A:509:GLU:H	1.99	0.64
1:A:793:SER:O	1:A:797:ARG:HG3	1.97	0.64
1:B:446:MET:HE3	1:B:537:TRP:CE3	2.32	0.64
1:B:629:THR:HG23	1:B:801:PRO:CB	2.28	0.64
1:A:630:THR:CB	1:A:969:GLY:HA3	2.20	0.64
1:B:614:THR:HG22	1:B:614:THR:O	1.98	0.64
1:B:500:GLN:OE1	1:B:545:GLN:HB2	1.98	0.64
1:B:444:PHE:HZ	1:B:447:GLU:HB2	1.62	0.64
1:A:303:LEU:CA	1:A:304:ARG:NH2	2.57	0.64
1:A:884:TYR:CE2	1:B:885:ARG:CB	2.73	0.64
1:B:602:LYS:O	1:B:956:ILE:O	2.13	0.64
1:B:603:ALA:CA	1:B:956:ILE:HB	2.27	0.64
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.63	0.64
1:B:507:THR:C	1:B:509:GLU:H	1.99	0.64
1:A:398:ARG:HH21	1:A:398:ARG:HA	1.62	0.63
1:A:444:PHE:HZ	1:A:447:GLU:HB2	1.62	0.63
1:A:614:THR:HG22	1:A:614:THR:O	1.98	0.63
1:A:905:HIS:HE1	1:B:1014:LEU:HD11	1.59	0.63
1:B:547:ARG:HH11	1:B:548:SER:N	1.97	0.63
1:B:780:HIS:CE1	1:B:782:ILE:HD12	2.34	0.63
1:B:214:GLN:HE22	1:B:550:LEU:C	2.00	0.63
1:A:1010:PHE:CZ	1:B:879:ASN:HB3	2.33	0.63
1:B:602:LYS:C	1:B:958:PHE:CB	2.66	0.63
1:A:269:MET:HB3	1:A:694:ARG:HH12	1.64	0.63
1:A:419:ILE:HG13	1:A:422:MET:SD	2.39	0.63
1:B:630:THR:CB	1:B:805:VAL:CG1	2.75	0.63
1:B:568:ARG:C	1:B:569:LEU:HD22	2.18	0.63
1:A:402:GLU:CG	1:A:536:ASN:OD1	2.46	0.63
1:B:602:LYS:C	1:B:958:PHE:HB2	2.17	0.63
1:A:780:HIS:CE1	1:A:782:ILE:HD12	2.33	0.62
1:B:235:LYS:HD3	1:B:235:LYS:H	1.64	0.62
1:A:301:ASP:O	1:A:304:ARG:CG	2.46	0.62
1:A:568:ARG:C	1:A:569:LEU:HD22	2.18	0.62
1:B:333:GLU:HG2	1:B:501:ILE:HG13	1.81	0.62
1:B:500:GLN:HE22	1:B:545:GLN:HB2	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:LEU:HD22	1:A:962:ARG:NH1	2.15	0.62
1:A:269:MET:HE3	1:A:687:LEU:CD1	2.28	0.62
1:B:459:ARG:HG2	1:B:459:ARG:HH11	1.63	0.62
1:A:810:THR:HG22	1:B:1001:MET:CE	2.29	0.62
1:B:629:THR:O	1:B:805:VAL:HG21	1.99	0.62
1:A:735:LYS:HD2	1:A:739:ARG:NH2	2.15	0.62
1:A:881:SER:OG	1:B:880:SER:C	2.37	0.61
1:B:450:LEU:HD12	1:B:461:ILE:HD12	1.83	0.61
1:B:342:LEU:CD2	1:B:550:LEU:HD11	1.94	0.61
1:B:367:GLN:O	1:B:371:GLU:HG2	2.01	0.61
1:A:547:ARG:NH1	1:A:547:ARG:HB2	2.16	0.61
1:A:905:HIS:CD2	1:B:1019:ARG:HH22	2.17	0.61
1:B:735:LYS:HD2	1:B:739:ARG:NH2	2.15	0.61
1:A:364:SER:HB3	1:A:370:LYS:HG2	1.82	0.61
1:B:260:LEU:HD22	1:B:264:GLU:HG3	1.83	0.61
1:B:341:ARG:HH12	1:B:535:ASN:HA	1.66	0.61
1:A:629:THR:HG21	1:A:973:GLN:HB2	1.83	0.60
1:A:260:LEU:HD22	1:A:264:GLU:HG3	1.83	0.60
1:A:364:SER:HB3	1:A:370:LYS:CG	2.32	0.60
1:A:450:LEU:HD12	1:A:461:ILE:HD12	1.83	0.60
1:B:777:LEU:HD23	1:B:854:ARG:HG3	1.83	0.60
1:A:304:ARG:NE	1:A:304:ARG:H	1.98	0.60
1:A:367:GLN:O	1:A:371:GLU:HG2	2.01	0.60
1:A:840:VAL:CG1	1:A:1012:LYS:HB3	2.32	0.60
1:A:905:HIS:CE1	1:B:1014:LEU:CD1	2.73	0.60
1:B:364:SER:HB3	1:B:370:LYS:CG	2.32	0.60
1:A:777:LEU:HD23	1:A:854:ARG:HG3	1.83	0.60
1:B:840:VAL:CG1	1:B:1012:LYS:HB3	2.32	0.60
1:B:917:ALA:HA	1:B:920:ARG:NH2	2.17	0.60
1:B:269:MET:CB	1:B:691:ASN:CG	2.69	0.59
1:A:885:ARG:CB	1:B:884:TYR:CE2	2.77	0.59
1:B:224:LYS:HG3	1:B:225:VAL:HG23	1.84	0.59
1:A:269:MET:HG2	1:A:691:ASN:CG	2.21	0.59
1:B:221:LEU:HD23	1:B:550:LEU:CD2	2.33	0.59
1:B:364:SER:HB3	1:B:370:LYS:HG2	1.83	0.59
1:A:1001:MET:CE	1:B:810:THR:HG22	2.32	0.59
1:B:456:LYS:H	1:B:456:LYS:HE3	1.67	0.59
1:B:630:THR:HG22	1:B:805:VAL:HG21	1.85	0.59
1:A:260:LEU:O	1:A:264:GLU:HG3	2.03	0.59
1:A:905:HIS:CD2	1:B:1019:ARG:NH2	2.70	0.59
1:B:428:ASN:ND2	1:B:487:GLU:N	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:LEU:HD13	1:B:905:HIS:NE2	2.18	0.59
1:B:272:GLU:HG3	1:B:625:ARG:NH2	2.17	0.58
1:A:575:TYR:HD2	1:A:651:PRO:HG2	1.69	0.58
1:B:644:ILE:HG23	1:B:689:VAL:HG13	1.85	0.58
1:A:629:THR:HG22	1:A:969:GLY:CA	2.33	0.58
1:B:575:TYR:HD2	1:B:651:PRO:HG2	1.69	0.58
1:B:260:LEU:O	1:B:264:GLU:HG3	2.03	0.58
1:A:644:ILE:HG23	1:A:689:VAL:HG13	1.85	0.58
1:B:258:LYS:HA	1:B:258:LYS:NZ	2.19	0.58
1:B:269:MET:HB3	1:B:691:ASN:CG	2.24	0.58
1:A:630:THR:CG2	1:A:969:GLY:CA	2.17	0.57
1:B:458:GLU:CD	1:B:458:GLU:O	2.42	0.57
1:B:269:MET:CB	1:B:691:ASN:OD1	2.45	0.57
1:A:428:ASN:ND2	1:A:487:GLU:N	2.51	0.57
1:B:456:LYS:H	1:B:456:LYS:CE	2.17	0.57
1:B:519:LYS:NZ	1:B:519:LYS:HB2	2.19	0.57
1:A:1014:LEU:HD11	1:B:905:HIS:NE2	2.19	0.57
1:A:506:ASP:OD1	1:A:510:TYR:CE2	2.57	0.57
1:A:629:THR:O	1:A:969:GLY:HA2	2.04	0.57
1:A:498:LYS:HB2	1:A:517:ILE:O	2.04	0.57
1:A:271:ASP:CG	1:A:273:GLY:H	2.08	0.57
1:B:276:HIS:CE1	1:B:365:GLU:H	2.22	0.57
1:B:497:ARG:H	1:B:498:LYS:HD3	1.70	0.57
1:A:905:HIS:NE2	1:B:1019:ARG:NH2	2.48	0.57
1:B:428:ASN:HD21	1:B:487:GLU:N	2.03	0.57
1:B:767:ARG:NH1	1:B:767:ARG:HB2	2.20	0.57
1:B:235:LYS:HD3	1:B:235:LYS:N	2.20	0.56
1:B:218:GLU:CG	1:B:550:LEU:C	2.74	0.56
1:A:1003:LYS:CE	1:B:929:PHE:CE1	2.84	0.56
1:A:419:ILE:HG13	1:A:422:MET:HB2	1.87	0.56
1:B:584:GLU:CD	1:B:953:LYS:HD2	2.25	0.56
1:A:269:MET:HE2	1:A:729:TRP:NE1	2.19	0.56
1:B:423:ASN:O	1:B:427:LYS:HD3	2.04	0.56
1:B:314:GLN:HE22	1:B:317:LYS:NZ	2.04	0.56
1:A:302:ILE:C	1:A:304:ARG:HE	2.09	0.56
1:A:456:LYS:HD2	1:A:457:HIS:CD2	2.39	0.56
1:A:860:GLN:HG3	1:A:900:ILE:HD13	1.87	0.56
1:B:269:MET:CE	1:B:691:ASN:N	2.66	0.56
1:A:276:HIS:CE1	1:A:365:GLU:H	2.22	0.56
1:A:419:ILE:CG1	1:A:422:MET:HB2	2.36	0.56
1:A:428:ASN:HD21	1:A:487:GLU:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLN:HE22	1:A:317:LYS:NZ	2.04	0.56
1:B:506:ASP:CG	1:B:508:ASN:HB3	2.24	0.56
1:A:929:PHE:CZ	1:B:1003:LYS:HE3	2.40	0.56
1:A:421:LYS:HZ1	1:A:425:ILE:HD11	1.72	0.55
1:B:221:LEU:HD23	1:B:550:LEU:HD23	1.88	0.55
1:B:602:LYS:CE	1:B:948:LEU:HD12	2.17	0.55
1:B:860:GLN:HG3	1:B:900:ILE:HD13	1.87	0.55
1:A:507:THR:O	1:A:509:GLU:N	2.39	0.55
1:A:611:GLU:HA	1:A:647:ARG:NH1	2.22	0.55
1:B:235:LYS:NZ	1:B:235:LYS:HB2	2.21	0.55
1:A:629:THR:HG21	1:A:969:GLY:O	2.00	0.55
1:B:342:LEU:CD1	1:B:550:LEU:CD2	2.74	0.55
1:B:403:SER:OG	1:B:539:ALA:HB1	2.06	0.55
1:B:601:ILE:O	1:B:958:PHE:HD2	1.87	0.55
1:B:269:MET:CA	1:B:691:ASN:ND2	2.69	0.55
1:A:302:ILE:O	1:A:304:ARG:CZ	2.55	0.55
1:B:269:MET:HA	1:B:691:ASN:ND2	2.22	0.55
1:B:504:LYS:HA	1:B:504:LYS:HE3	1.89	0.55
1:B:547:ARG:O	1:B:547:ARG:HD2	2.06	0.55
1:A:269:MET:SD	1:A:687:LEU:HD21	2.47	0.54
1:A:999:ASN:ND2	1:B:942:GLU:CD	2.60	0.54
1:A:766:SER:OG	1:A:778:THR:HB	2.07	0.54
1:B:766:SER:OG	1:B:778:THR:HB	2.08	0.54
1:B:947:VAL:HG11	1:B:954:GLU:CG	2.37	0.54
1:A:446:MET:HE2	1:A:463:LEU:HD12	1.89	0.54
1:A:499:VAL:CG2	1:A:517:ILE:HB	2.25	0.54
1:B:221:LEU:CD1	1:B:549:THR:OG1	2.54	0.54
1:B:629:THR:HG21	1:B:968:THR:HG21	1.89	0.54
1:B:630:THR:HG22	1:B:805:VAL:CG1	2.38	0.54
1:B:519:LYS:O	1:B:519:LYS:HD3	2.06	0.54
1:B:630:THR:HG22	1:B:805:VAL:HG22	1.88	0.54
1:B:547:ARG:HH11	1:B:547:ARG:HB3	1.73	0.54
1:A:1036:LYS:HD3	1:A:1037:SER:O	2.08	0.54
1:B:272:GLU:HG3	1:B:625:ARG:HH22	1.71	0.54
1:A:397:LYS:HB3	1:A:397:LYS:NZ	2.24	0.53
1:A:568:ARG:HG3	1:A:568:ARG:HH21	1.73	0.53
1:B:456:LYS:HG2	1:B:457:HIS:ND1	2.22	0.53
1:B:217:ARG:NH2	1:B:548:SER:C	2.44	0.53
1:B:611:GLU:HA	1:B:647:ARG:NH1	2.22	0.53
1:A:511:LYS:O	1:A:511:LYS:HD2	2.09	0.53
1:A:402:GLU:HG3	1:A:536:ASN:OD1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:HD2	1:B:518:LEU:HD13	1.89	0.53
1:B:498:LYS:CG	1:B:518:LEU:HD13	2.33	0.53
1:A:269:MET:CG	1:A:691:ASN:ND2	2.33	0.53
1:A:498:LYS:CG	1:A:518:LEU:HD23	2.38	0.53
1:B:603:ALA:HA	1:B:956:ILE:HB	1.91	0.53
1:A:304:ARG:NH1	1:A:307:PHE:HB2	2.09	0.53
1:A:421:LYS:NZ	1:A:425:ILE:HD11	2.24	0.53
1:B:604:GLY:H	1:B:956:ILE:CG1	2.22	0.53
1:A:394:SER:O	1:A:398:ARG:HG2	2.09	0.53
1:A:947:VAL:HG11	1:A:954:GLU:CG	2.37	0.53
1:B:695:HIS:CD2	1:B:699:HIS:HD2	2.27	0.53
1:B:963:LYS:HZ2	1:B:963:LYS:HB3	1.73	0.53
1:B:245:ILE:HD11	1:B:314:GLN:HG2	1.91	0.53
1:B:500:GLN:CD	1:B:545:GLN:HB2	2.29	0.53
1:A:269:MET:CE	1:A:729:TRP:NE1	2.68	0.52
1:A:653:PRO:HD3	1:A:678:ARG:NH1	2.24	0.52
1:A:304:ARG:NH2	1:A:399:ARG:HH11	1.92	0.52
1:A:245:ILE:HD11	1:A:314:GLN:HG2	1.91	0.52
1:B:1036:LYS:NZ	1:B:1036:LYS:HB2	2.23	0.52
1:B:653:PRO:HD3	1:B:678:ARG:NH1	2.24	0.52
1:B:258:LYS:HA	1:B:258:LYS:HZ2	1.74	0.52
1:B:449:THR:HG23	1:B:458:GLU:OE1	2.09	0.52
1:B:568:ARG:HG3	1:B:568:ARG:HH21	1.73	0.52
1:B:568:ARG:O	1:B:569:LEU:HD13	2.09	0.52
1:A:905:HIS:NE2	1:B:1019:ARG:CZ	2.72	0.52
1:B:311:PHE:O	1:B:315:LEU:HD13	2.09	0.52
1:A:519:LYS:CD	1:A:519:LYS:H	2.22	0.52
1:A:518:LEU:HB2	1:A:521:GLU:HB2	1.91	0.52
1:A:684:PRO:O	1:A:688:ARG:HG2	2.10	0.52
1:A:568:ARG:O	1:A:569:LEU:HD13	2.09	0.52
1:A:695:HIS:CD2	1:A:699:HIS:HD2	2.27	0.52
1:A:780:HIS:HE1	1:A:782:ILE:HD12	1.74	0.52
1:A:630:THR:HG22	1:A:969:GLY:C	2.19	0.51
1:B:547:ARG:HH11	1:B:547:ARG:C	2.13	0.51
1:B:511:LYS:O	1:B:511:LYS:HD2	2.09	0.51
1:A:302:ILE:C	1:A:304:ARG:HH21	2.13	0.51
1:B:601:ILE:O	1:B:958:PHE:CG	2.63	0.51
1:B:890:PHE:HA	1:B:893:ILE:HD12	1.93	0.51
1:A:311:PHE:O	1:A:315:LEU:HD13	2.09	0.51
1:B:337:TYR:CD1	1:B:538:MET:HE2	2.42	0.51
1:B:601:ILE:C	1:B:958:PHE:HB3	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:PRO:O	1:B:688:ARG:HG2	2.10	0.51
1:A:780:HIS:HE1	1:A:782:ILE:CD1	2.24	0.50
1:A:884:TYR:CZ	1:B:885:ARG:HD2	2.45	0.50
1:B:507:THR:O	1:B:509:GLU:N	2.40	0.50
1:A:727:LYS:O	1:A:731:GLU:HG3	2.12	0.50
1:B:602:LYS:CA	1:B:958:PHE:CB	2.89	0.50
1:A:890:PHE:HA	1:A:893:ILE:HD12	1.93	0.50
1:A:206:LYS:NZ	1:A:206:LYS:HB3	2.26	0.50
1:A:304:ARG:CZ	1:A:304:ARG:N	2.74	0.50
1:A:304:ARG:HD3	1:A:307:PHE:CB	2.36	0.50
1:B:446:MET:HE2	1:B:463:LEU:HD12	1.94	0.50
1:B:896:ARG:HH11	1:B:896:ARG:HG2	1.77	0.50
1:A:648:PHE:HE2	1:A:722:ARG:NH1	2.09	0.50
1:A:896:ARG:HG2	1:A:896:ARG:HH11	1.77	0.50
1:B:630:THR:HB	1:B:805:VAL:CG1	2.41	0.50
1:B:727:LYS:O	1:B:731:GLU:HG3	2.12	0.50
1:A:399:ARG:O	1:A:402:GLU:HB3	2.12	0.50
1:B:399:ARG:O	1:B:402:GLU:HB3	2.12	0.50
1:B:780:HIS:HE1	1:B:782:ILE:HD12	1.74	0.50
1:A:905:HIS:HE1	1:B:1010:PHE:HE2	1.60	0.50
1:B:780:HIS:HE1	1:B:782:ILE:CD1	2.24	0.50
1:A:999:ASN:CB	1:B:938:LEU:HD21	2.38	0.49
1:A:926:CYS:HA	1:A:979:TYR:OH	2.13	0.49
1:B:235:LYS:HZ3	1:B:235:LYS:HB2	1.77	0.49
1:B:496:MET:CA	1:B:498:LYS:HZ3	2.17	0.49
1:B:579:GLU:O	1:B:608:LYS:HE2	2.12	0.49
1:B:648:PHE:HE2	1:B:722:ARG:NH1	2.09	0.49
1:A:579:GLU:O	1:A:608:LYS:HE2	2.12	0.49
1:B:446:MET:CE	1:B:463:LEU:HD12	2.43	0.49
1:B:498:LYS:N	1:B:498:LYS:HD3	2.26	0.49
1:B:926:CYS:HA	1:B:979:TYR:OH	2.13	0.49
1:A:500:GLN:HE22	1:A:516:ILE:CG1	2.25	0.49
1:A:304:ARG:H	1:A:304:ARG:HE	1.60	0.49
1:A:458:GLU:H	1:A:458:GLU:CD	2.16	0.49
1:A:720:THR:O	1:A:722:ARG:HD3	2.13	0.49
1:B:337:TYR:CD1	1:B:538:MET:CE	2.95	0.49
1:B:268:GLU:OE1	1:B:619:ALA:CB	2.34	0.49
1:B:808:VAL:HG11	1:B:817:ASN:HB3	1.95	0.49
1:A:446:MET:CE	1:A:463:LEU:HD12	2.42	0.49
1:A:613:LEU:HD11	1:A:624:VAL:HA	1.94	0.49
1:A:1003:LYS:HE2	1:B:929:PHE:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE3	1:A:729:TRP:CE2	2.15	0.48
1:B:499:VAL:HG23	1:B:545:GLN:HE22	1.79	0.48
1:B:269:MET:SD	1:B:687:LEU:HG	2.53	0.48
1:B:720:THR:O	1:B:722:ARG:HD3	2.13	0.48
1:A:808:VAL:HG11	1:A:817:ASN:HB3	1.95	0.48
1:B:603:ALA:C	1:B:956:ILE:HB	2.31	0.48
1:A:575:TYR:O	1:A:576:ARG:HG2	2.14	0.48
1:A:586:ILE:HG13	1:A:608:LYS:HG2	1.94	0.48
1:B:613:LEU:HD11	1:B:624:VAL:HA	1.94	0.48
1:A:303:LEU:C	1:A:304:ARG:NH2	2.66	0.48
1:B:202:TYR:CE2	1:B:206:LYS:HD2	2.48	0.48
1:B:603:ALA:CA	1:B:956:ILE:CB	2.89	0.48
1:A:265:ASP:HB3	1:A:687:LEU:CD2	2.41	0.48
1:B:456:LYS:N	1:B:456:LYS:HE3	2.28	0.48
1:B:398:ARG:CG	1:B:532:GLU:CD	2.72	0.48
1:A:568:ARG:HH12	1:A:616:HIS:CE1	2.32	0.48
1:B:576:ARG:HB3	1:B:578:ALA:H	1.78	0.48
1:B:260:LEU:HD22	1:B:264:GLU:CG	2.44	0.48
1:B:498:LYS:HG2	1:B:517:ILE:O	2.14	0.48
1:B:496:MET:SD	1:B:498:LYS:NZ	2.86	0.48
1:A:423:ASN:O	1:A:427:LYS:HG3	2.14	0.48
1:A:443:GLU:HG2	1:A:444:PHE:N	2.29	0.48
1:A:735:LYS:HE3	1:A:739:ARG:HH21	1.79	0.48
1:B:543:SER:HA	1:B:550:LEU:HD12	1.96	0.48
1:B:586:ILE:HG13	1:B:608:LYS:HG2	1.94	0.47
1:B:963:LYS:NZ	1:B:963:LYS:HB3	2.28	0.47
1:A:941:GLU:HA	1:A:960:LYS:HE3	1.96	0.47
1:B:402:GLU:OE2	1:B:536:ASN:CG	2.53	0.47
1:B:500:GLN:C	1:B:501:ILE:HD12	2.35	0.47
1:B:676:ARG:HG2	1:B:676:ARG:HH11	1.79	0.47
1:A:500:GLN:C	1:A:501:ILE:HD12	2.35	0.47
1:A:269:MET:HG3	1:A:691:ASN:HD21	1.61	0.47
1:B:584:GLU:CG	1:B:953:LYS:CE	2.92	0.47
1:B:941:GLU:HA	1:B:960:LYS:HE3	1.96	0.47
1:A:547:ARG:HH11	1:A:547:ARG:CB	2.27	0.47
1:A:576:ARG:HB3	1:A:578:ALA:H	1.78	0.47
1:B:506:ASP:OD2	1:B:510:TYR:CE2	2.67	0.47
1:B:575:TYR:O	1:B:576:ARG:HG2	2.14	0.47
1:B:735:LYS:HE3	1:B:739:ARG:HH21	1.79	0.47
1:A:735:LYS:O	1:A:735:LYS:HD3	2.15	0.47
1:A:519:LYS:HD3	1:A:519:LYS:N	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ARG:HH21	1:B:310:ARG:HG2	1.79	0.47
1:B:499:VAL:HG11	1:B:517:ILE:HD12	1.97	0.47
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.80	0.47
1:A:304:ARG:HD2	1:A:307:PHE:N	2.30	0.47
1:A:314:GLN:HE21	1:A:317:LYS:HZ3	1.62	0.47
1:A:935:THR:CB	1:B:1004:GLU:OE2	2.58	0.47
1:B:457:HIS:NE2	1:B:459:ARG:NH1	2.63	0.47
1:A:260:LEU:HD22	1:A:264:GLU:CG	2.44	0.47
1:B:807:SER:HA	1:B:809:TRP:CZ3	2.50	0.47
1:B:626:THR:HG23	1:B:965:ALA:HB2	1.96	0.47
1:B:446:MET:CE	1:B:540:ALA:HB3	2.45	0.47
1:B:568:ARG:HH12	1:B:616:HIS:CE1	2.32	0.47
1:A:630:THR:HG21	1:A:966:GLU:O	2.15	0.46
1:A:421:LYS:O	1:A:425:ILE:HG13	2.15	0.46
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.15	0.46
1:B:421:LYS:O	1:B:425:ILE:HG13	2.15	0.46
1:A:1014:LEU:HD11	1:B:905:HIS:HE1	1.75	0.46
1:A:202:TYR:CD2	1:A:206:LYS:HD2	2.50	0.46
1:A:530:SER:OG	1:A:533:GLU:HG3	2.15	0.46
1:A:446:MET:CE	1:A:540:ALA:HB3	2.45	0.46
1:A:676:ARG:HG2	1:A:676:ARG:HH11	1.79	0.46
1:A:507:THR:C	1:A:509:GLU:N	2.67	0.46
1:A:510:TYR:O	1:A:510:TYR:CD1	2.69	0.46
1:A:630:THR:O	1:A:965:ALA:HB1	2.14	0.46
1:A:905:HIS:CG	1:B:1019:ARG:CZ	2.98	0.46
1:B:498:LYS:CG	1:B:517:ILE:O	2.64	0.46
1:A:605:THR:HG22	1:A:607:ILE:H	1.80	0.46
1:A:506:ASP:OD2	1:A:506:ASP:O	2.33	0.46
1:B:735:LYS:CE	1:B:739:ARG:HH21	2.28	0.46
1:A:398:ARG:CA	1:A:398:ARG:HH21	2.28	0.46
1:A:735:LYS:CE	1:A:739:ARG:HH21	2.28	0.46
1:B:457:HIS:CD2	1:B:472:LYS:HG3	2.51	0.46
1:B:269:MET:HE3	1:B:691:ASN:N	2.13	0.46
1:A:519:LYS:O	1:A:521:GLU:HG2	2.16	0.46
1:A:807:SER:HA	1:A:809:TRP:CZ3	2.50	0.46
1:A:258:LYS:HE2	1:A:286:LEU:CD2	2.40	0.46
1:A:879:ASN:CB	1:B:1010:PHE:CZ	2.98	0.46
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.80	0.46
1:B:272:GLU:CG	1:B:625:ARG:NH2	2.79	0.46
1:B:507:THR:C	1:B:509:GLU:N	2.67	0.46
1:B:510:TYR:CD1	1:B:510:TYR:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:HA	1:A:228:GLU:OE1	2.15	0.45
1:A:458:GLU:HG2	1:A:458:GLU:O	2.17	0.45
1:B:341:ARG:HG3	1:B:539:ALA:HB1	1.07	0.45
1:B:847:GLU:HG2	1:B:1035:LEU:HD21	1.98	0.45
1:A:269:MET:SD	1:A:687:LEU:CD1	2.95	0.45
1:A:500:GLN:NE2	1:A:516:ILE:HG12	2.32	0.45
1:B:605:THR:HG22	1:B:607:ILE:H	1.80	0.45
1:B:735:LYS:HD3	1:B:735:LYS:O	2.15	0.45
1:A:202:TYR:CE2	1:A:206:LYS:HD2	2.51	0.45
1:A:497:ARG:NH2	1:A:519:LYS:HB3	2.31	0.45
1:B:584:GLU:HG2	1:B:953:LYS:HG3	1.97	0.45
1:B:603:ALA:CB	1:B:955:LEU:C	2.62	0.45
1:A:629:THR:HG23	1:A:969:GLY:O	2.04	0.45
1:B:254:GLU:O	1:B:258:LYS:HG2	2.17	0.45
1:B:499:VAL:CG1	1:B:517:ILE:HD12	2.46	0.45
1:B:506:ASP:C	1:B:508:ASN:N	2.68	0.45
1:B:519:LYS:HD3	1:B:520:ASP:OD2	2.17	0.45
1:A:398:ARG:HB3	1:A:398:ARG:NH2	2.31	0.45
1:A:470:CYS:HB2	1:A:492:GLU:HB2	1.99	0.45
1:A:682:ILE:HG23	1:A:686:GLN:HE21	1.82	0.45
1:A:609:LEU:HD21	1:A:962:ARG:NH1	2.32	0.45
1:B:202:TYR:CD2	1:B:206:LYS:HD2	2.52	0.45
1:B:650:ILE:HA	1:B:651:PRO:HD3	1.82	0.45
1:A:929:PHE:CE1	1:B:1003:LYS:CE	2.89	0.45
1:B:314:GLN:HE21	1:B:317:LYS:HZ3	1.64	0.45
1:B:767:ARG:HD3	1:B:767:ARG:N	2.31	0.45
1:A:389:LYS:HD3	1:A:389:LYS:O	2.16	0.45
1:B:421:LYS:NZ	1:B:425:ILE:HG13	2.32	0.45
1:A:471:CYS:HB3	1:A:488:TYR:HB3	2.00	0.44
1:B:471:CYS:HB3	1:B:488:TYR:HB3	1.99	0.44
1:B:574:VAL:O	1:B:574:VAL:HG12	2.17	0.44
1:A:574:VAL:O	1:A:574:VAL:HG12	2.17	0.44
1:A:506:ASP:C	1:A:508:ASN:N	2.68	0.44
1:A:724:LYS:NZ	1:A:727:LYS:NZ	2.65	0.44
1:B:547:ARG:HD2	1:B:547:ARG:C	2.37	0.44
1:A:456:LYS:HD3	1:A:456:LYS:O	2.18	0.44
1:A:609:LEU:HD21	1:A:962:ARG:HH11	1.82	0.44
1:A:885:ARG:HD2	1:B:884:TYR:CZ	2.52	0.44
1:B:724:LYS:NZ	1:B:727:LYS:NZ	2.65	0.44
1:A:568:ARG:NH1	1:A:616:HIS:CE1	2.86	0.44
1:B:676:ARG:HD3	1:B:676:ARG:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:317:LYS:NZ	2.51	0.44
1:A:847:GLU:HG2	1:A:1035:LEU:HD21	1.98	0.44
1:A:394:SER:HA	1:A:397:LYS:HZ2	1.83	0.44
1:A:676:ARG:HD3	1:A:676:ARG:N	2.33	0.44
1:B:298:TYR:CE2	1:B:302:ILE:HG13	2.52	0.44
1:B:402:GLU:OE2	1:B:535:ASN:HB2	2.18	0.44
1:B:341:ARG:NH2	1:B:536:ASN:C	2.71	0.44
1:A:364:SER:HB3	1:A:370:LYS:HG3	1.99	0.44
1:A:500:GLN:HE22	1:A:516:ILE:HG12	1.82	0.44
1:A:722:ARG:N	1:A:722:ARG:HD3	2.33	0.44
1:B:457:HIS:NE2	1:B:472:LYS:HD2	2.33	0.44
1:B:498:LYS:CD	1:B:518:LEU:HD13	2.47	0.44
1:B:568:ARG:NH1	1:B:616:HIS:CE1	2.86	0.44
1:B:519:LYS:O	1:B:520:ASP:CG	2.56	0.43
1:A:298:TYR:CE2	1:A:302:ILE:HG13	2.52	0.43
1:A:457:HIS:CD2	1:A:472:LYS:NZ	2.86	0.43
1:A:609:LEU:CD2	1:A:962:ARG:HH11	2.31	0.43
1:B:470:CYS:HB2	1:B:492:GLU:HB2	1.99	0.43
1:A:248:ARG:NE	1:A:248:ARG:HA	2.33	0.43
1:A:942:GLU:OE2	1:B:999:ASN:ND2	2.52	0.43
1:B:364:SER:HB3	1:B:370:LYS:HG3	1.99	0.43
1:B:682:ILE:HG23	1:B:686:GLN:HE21	1.82	0.43
1:B:872:LEU:HD12	1:B:929:PHE:CG	2.53	0.43
1:B:947:VAL:HG12	1:B:949:LYS:HZ2	1.83	0.43
1:B:358:LYS:HE2	1:B:358:LYS:HA	2.01	0.43
1:B:422:MET:HG2	1:B:464:PHE:HE2	1.83	0.43
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.32	0.43
1:A:647:ARG:HD2	1:A:647:ARG:HA	1.92	0.43
1:B:248:ARG:NE	1:B:248:ARG:HA	2.33	0.43
1:A:872:LEU:HD12	1:A:929:PHE:CG	2.53	0.43
1:A:1010:PHE:HE2	1:B:905:HIS:HE1	1.66	0.43
1:B:236:LEU:O	1:B:317:LYS:NZ	2.51	0.43
1:B:292:PHE:HE2	1:B:353:TYR:CE2	2.36	0.43
1:A:293:ASP:N	1:A:294:PRO:CD	2.82	0.43
1:A:208:PHE:CE1	1:A:353:TYR:HE1	2.37	0.43
1:B:208:PHE:CE1	1:B:353:TYR:HE1	2.37	0.43
1:B:722:ARG:N	1:B:722:ARG:HD3	2.33	0.43
1:A:339:LEU:N	1:A:340:PRO:HD2	2.34	0.43
1:A:422:MET:HG2	1:A:464:PHE:HE2	1.83	0.43
1:B:221:LEU:HD22	1:B:549:THR:C	2.31	0.43
1:B:500:GLN:OE1	1:B:541:LEU:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASP:OD1	1:A:510:TYR:CD2	2.72	0.42
1:A:629:THR:CG2	1:A:969:GLY:C	2.67	0.42
1:B:293:ASP:N	1:B:294:PRO:CD	2.82	0.42
1:B:339:LEU:N	1:B:340:PRO:HD2	2.34	0.42
1:B:402:GLU:CD	1:B:535:ASN:C	2.75	0.42
1:B:422:MET:HG2	1:B:464:PHE:CE2	2.54	0.42
1:A:1019:ARG:CZ	1:B:905:HIS:CG	2.99	0.42
1:A:271:ASP:OD2	1:A:273:GLY:N	2.51	0.42
1:A:422:MET:HG2	1:A:464:PHE:CE2	2.54	0.42
1:B:341:ARG:NH2	1:B:539:ALA:H	2.14	0.42
1:A:341:ARG:NH2	1:A:536:ASN:HA	2.34	0.42
1:A:292:PHE:HE2	1:A:353:TYR:CE2	2.36	0.42
1:A:419:ILE:O	1:A:419:ILE:HG12	2.19	0.42
1:B:337:TYR:C	1:B:542:ILE:HG13	2.39	0.42
1:B:630:THR:CG2	1:B:805:VAL:HG11	2.49	0.42
1:A:500:GLN:NE2	1:A:514:PHE:HD1	2.18	0.42
1:A:777:LEU:HA	1:A:854:ARG:NH1	2.35	0.42
1:A:325:GLN:HG3	1:A:332:LYS:HD2	2.02	0.42
1:A:395:LEU:HD22	1:A:395:LEU:N	2.35	0.42
1:B:516:ILE:HG22	1:B:518:LEU:HD22	2.01	0.42
1:A:764:HIS:CG	1:A:765:ILE:N	2.88	0.42
1:A:852:VAL:HG11	1:A:893:ILE:HD11	2.01	0.42
1:A:500:GLN:CD	1:A:516:ILE:HG12	2.38	0.42
1:A:764:HIS:CG	1:A:765:ILE:H	2.38	0.42
1:B:506:ASP:OD1	1:B:510:TYR:CG	2.73	0.42
1:B:852:VAL:HG11	1:B:893:ILE:HD11	2.01	0.42
1:B:603:ALA:HA	1:B:956:ILE:CB	2.48	0.42
1:A:572:ALA:O	1:A:573:ASP:HB3	2.20	0.42
1:A:935:THR:OG1	1:B:1004:GLU:CG	2.68	0.42
1:B:777:LEU:HA	1:B:854:ARG:NH1	2.34	0.42
1:B:395:LEU:HD22	1:B:395:LEU:N	2.35	0.42
1:B:585:ASN:HB3	1:B:608:LYS:HG2	2.02	0.42
1:B:764:HIS:CG	1:B:765:ILE:N	2.88	0.42
1:A:304:ARG:CZ	1:A:399:ARG:NH1	2.65	0.41
1:A:465:ASP:HA	1:A:544:LEU:HD21	2.02	0.41
1:A:879:ASN:CG	1:B:1010:PHE:CZ	2.93	0.41
1:B:572:ALA:O	1:B:573:ASP:HB3	2.20	0.41
1:A:780:HIS:HE1	1:A:782:ILE:CG1	2.33	0.41
1:B:420:LYS:O	1:B:424:GLU:HG2	2.20	0.41
1:B:780:HIS:HE1	1:B:782:ILE:CG1	2.33	0.41
1:B:630:THR:CG2	1:B:805:VAL:CG1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HG3	1:A:897:GLN:N	2.36	0.41
1:B:325:GLN:HG3	1:B:332:LYS:HD2	2.02	0.41
1:B:506:ASP:O	1:B:506:ASP:OD1	2.39	0.41
1:A:544:LEU:CA	1:A:547:ARG:HH12	2.26	0.41
1:B:465:ASP:HA	1:B:544:LEU:HD21	2.02	0.41
1:B:446:MET:HE2	1:B:540:ALA:HB3	2.01	0.41
1:B:852:VAL:CG1	1:B:893:ILE:HD11	2.51	0.41
1:A:880:SER:CA	1:B:881:SER:HG	2.34	0.41
1:B:896:ARG:HG3	1:B:897:GLN:N	2.36	0.41
1:A:459:ARG:NE	1:A:492:GLU:OE1	2.54	0.41
1:A:852:VAL:CG1	1:A:893:ILE:HD11	2.50	0.41
1:B:518:LEU:HB2	1:B:521:GLU:HB2	2.02	0.41
1:B:600:ILE:HG23	1:B:962:ARG:HH12	1.77	0.41
1:A:295:TYR:CD1	1:A:350:CYS:HB2	2.55	0.41
1:A:371:GLU:HA	1:A:371:GLU:OE1	2.21	0.41
1:B:519:LYS:HZ2	1:B:519:LYS:HB2	1.86	0.41
1:A:389:LYS:HD3	1:A:389:LYS:C	2.41	0.41
1:A:923:ASN:HA	1:A:924:PRO:HD2	1.85	0.41
1:A:630:THR:HG22	1:A:969:GLY:HA3	0.52	0.41
1:A:1004:GLU:CG	1:B:935:THR:OG1	2.68	0.41
1:B:212:ILE:CG2	1:B:260:LEU:HG	2.51	0.41
1:B:295:TYR:CD1	1:B:350:CYS:HB2	2.55	0.41
1:B:547:ARG:NH1	1:B:548:SER:N	2.64	0.41
1:B:640:LEU:HD13	1:B:696:TRP:CZ3	2.56	0.41
1:A:212:ILE:CG2	1:A:260:LEU:HG	2.51	0.40
1:B:244:ASN:HB3	1:B:310:ARG:CZ	2.50	0.40
1:B:371:GLU:HA	1:B:371:GLU:OE1	2.21	0.40
1:B:459:ARG:NE	1:B:492:GLU:OE1	2.54	0.40
1:A:585:ASN:HB3	1:A:608:LYS:HG2	2.02	0.40
1:B:421:LYS:HZ3	1:B:425:ILE:HG13	1.84	0.40
1:A:641:LEU:O	1:A:645:ILE:HG13	2.21	0.40
1:A:506:ASP:C	1:A:508:ASN:H	2.25	0.40
1:A:568:ARG:NH1	1:A:681:TYR:CD2	2.88	0.40
1:B:498:LYS:HB2	1:B:517:ILE:O	2.20	0.40
1:B:506:ASP:C	1:B:508:ASN:H	2.25	0.40
1:B:576:ARG:HD3	1:B:577:PHE:H	1.87	0.40
1:B:629:THR:HG23	1:B:801:PRO:HB3	1.99	0.40

All (122) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:OD2	1:B:300:ARG:NE[2_765]	0.38	1.82
1:A:894:PRO:C	1:B:575:TYR:OH[3_755]	0.54	1.66
1:A:949:LYS:CA	1:B:573:ASP:OD2[1_655]	0.56	1.64
1:A:953:LYS:CA	1:B:574:VAL:CG2[1_655]	0.66	1.54
1:A:953:LYS:N	1:B:574:VAL:CA[1_655]	0.67	1.53
1:A:953:LYS:CG	1:B:574:VAL:CG1[1_655]	0.72	1.48
1:A:949:LYS:CB	1:B:573:ASP:CG[1_655]	0.74	1.46
1:A:895:SER:N	1:B:575:TYR:CZ[3_755]	0.75	1.45
1:A:575:TYR:CE2	1:B:895:SER:O[3_845]	0.76	1.44
1:A:521:GLU:OE2	1:B:727:LYS:NZ[3_855]	0.84	1.36
1:A:953:LYS:CA	1:B:574:VAL:CB[1_655]	0.97	1.23
1:A:952:GLY:CA	1:B:575:TYR:N[1_655]	0.98	1.22
1:A:953:LYS:C	1:B:574:VAL:CG2[1_655]	0.98	1.22
1:A:952:GLY:C	1:B:574:VAL:CA[1_655]	1.06	1.14
1:A:575:TYR:OH	1:B:898:LYS:N[3_845]	1.12	1.08
1:A:953:LYS:N	1:B:574:VAL:CB[1_655]	1.12	1.08
1:A:288:GLU:O	1:B:389:LYS:NZ[2_765]	1.17	1.03
1:A:575:TYR:CE1	1:B:898:LYS:C[3_845]	1.17	1.03
1:A:575:TYR:OH	1:B:897:GLN:C[3_845]	1.18	1.02
1:A:651:PRO:CB	1:B:899:LYS:NZ[3_845]	1.18	1.02
1:A:952:GLY:C	1:B:574:VAL:N[1_655]	1.18	1.02
1:A:949:LYS:CB	1:B:573:ASP:OD2[1_655]	1.20	1.00
1:A:575:TYR:CE1	1:B:898:LYS:CA[3_845]	1.22	0.98
1:A:293:ASP:CG	1:B:300:ARG:NE[2_765]	1.23	0.97
1:A:953:LYS:CB	1:B:574:VAL:CG1[1_655]	1.25	0.95
1:A:895:SER:N	1:B:575:TYR:CE1[3_755]	1.30	0.90
1:A:895:SER:OG	1:B:575:TYR:CD1[3_755]	1.30	0.90
1:A:521:GLU:OE2	1:B:727:LYS:CE[3_855]	1.31	0.89
1:A:293:ASP:OD2	1:B:300:ARG:CZ[2_765]	1.32	0.88
1:A:894:PRO:CA	1:B:575:TYR:OH[3_755]	1.36	0.84
1:A:894:PRO:C	1:B:575:TYR:CZ[3_755]	1.42	0.78
1:A:288:GLU:C	1:B:389:LYS:NZ[2_765]	1.42	0.78
1:A:517:ILE:CG2	1:A:1044:ASN:ND2[1_655]	1.43	0.77
1:A:895:SER:N	1:B:575:TYR:OH[3_755]	1.45	0.75
1:A:952:GLY:CA	1:B:574:VAL:C[1_655]	1.46	0.74
1:A:951:HIS:O	1:B:574:VAL:O[1_655]	1.49	0.71
1:A:651:PRO:CG	1:B:899:LYS:NZ[3_845]	1.50	0.70
1:A:575:TYR:CE1	1:B:899:LYS:N[3_845]	1.53	0.67
1:A:575:TYR:CZ	1:B:898:LYS:N[3_845]	1.54	0.66
1:A:894:PRO:O	1:B:575:TYR:OH[3_755]	1.54	0.66
1:A:575:TYR:CD2	1:B:895:SER:O[3_845]	1.55	0.65
1:A:953:LYS:CD	1:B:574:VAL:CG1[1_655]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:LYS:C	1:B:573:ASP:OD2[1_655]	1.58	0.62
1:A:953:LYS:N	1:B:574:VAL:N[1_655]	1.62	0.58
1:A:949:LYS:CB	1:B:573:ASP:OD1[1_655]	1.62	0.58
1:A:952:GLY:C	1:B:574:VAL:C[1_655]	1.63	0.57
1:A:952:GLY:CA	1:B:574:VAL:N[1_655]	1.65	0.55
1:A:575:TYR:CE1	1:B:898:LYS:CB[3_845]	1.65	0.55
1:A:521:GLU:CD	1:B:727:LYS:NZ[3_855]	1.72	0.48
1:A:895:SER:OG	1:B:575:TYR:CG[3_755]	1.73	0.47
1:A:521:GLU:CA	1:B:724:LYS:NZ[3_855]	1.73	0.47
1:A:575:TYR:CD2	1:B:899:LYS:CD[3_845]	1.73	0.47
1:A:575:TYR:CG	1:B:899:LYS:CD[3_845]	1.73	0.47
1:A:575:TYR:CZ	1:B:899:LYS:N[3_845]	1.74	0.46
1:A:288:GLU:O	1:B:389:LYS:CE[2_765]	1.74	0.46
1:A:949:LYS:CA	1:B:573:ASP:CG[1_655]	1.74	0.46
1:A:949:LYS:CB	1:B:573:ASP:CB[1_655]	1.74	0.46
1:A:575:TYR:CD2	1:B:899:LYS:CE[3_845]	1.77	0.43
1:A:521:GLU:OE2	1:B:727:LYS:CD[3_855]	1.77	0.43
1:A:575:TYR:OH	1:B:897:GLN:CA[3_845]	1.79	0.41
1:A:952:GLY:C	1:B:574:VAL:CB[1_655]	1.80	0.40
1:A:954:GLU:N	1:B:574:VAL:CG2[1_655]	1.80	0.40
1:A:951:HIS:O	1:B:574:VAL:C[1_655]	1.80	0.40
1:A:293:ASP:OD2	1:B:300:ARG:CD[2_765]	1.80	0.40
1:A:289:GLU:N	1:B:389:LYS:NZ[2_765]	1.80	0.40
1:A:575:TYR:CZ	1:B:895:SER:O[3_845]	1.81	0.39
1:A:651:PRO:CG	1:B:899:LYS:CE[3_845]	1.83	0.37
1:A:952:GLY:CA	1:B:574:VAL:CA[1_655]	1.83	0.37
1:A:952:GLY:N	1:B:575:TYR:N[1_655]	1.84	0.36
1:A:952:GLY:N	1:B:573:ASP:O[1_655]	1.86	0.34
1:A:953:LYS:N	1:B:574:VAL:CG2[1_655]	1.87	0.33
1:A:953:LYS:CB	1:B:574:VAL:CB[1_655]	1.87	0.33
1:A:575:TYR:CB	1:B:899:LYS:CD[3_845]	1.88	0.32
1:A:949:LYS:CG	1:B:573:ASP:CB[1_655]	1.89	0.31
1:A:953:LYS:CA	1:B:574:VAL:CG1[1_655]	1.90	0.30
1:A:575:TYR:CE2	1:B:895:SER:C[3_845]	1.90	0.30
1:A:293:ASP:CG	1:B:300:ARG:CZ[2_765]	1.91	0.29
1:A:952:GLY:N	1:B:574:VAL:C[1_655]	1.92	0.28
1:A:575:TYR:OH	1:B:897:GLN:N[3_845]	1.93	0.27
1:A:575:TYR:CE1	1:B:898:LYS:N[3_845]	1.94	0.26
1:A:895:SER:N	1:B:575:TYR:CE2[3_755]	1.94	0.26
1:A:894:PRO:CA	1:B:575:TYR:CZ[3_755]	1.96	0.24
1:A:575:TYR:CD1	1:B:898:LYS:CB[3_845]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:LYS:CB	1:B:574:VAL:CG2[1_655]	1.97	0.23
1:A:895:SER:CA	1:B:575:TYR:CE1[3_755]	1.97	0.23
1:A:949:LYS:CD	1:B:573:ASP:CB[1_655]	1.98	0.22
1:A:949:LYS:N	1:B:573:ASP:OD2[1_655]	1.99	0.21
1:A:289:GLU:OE1	1:B:389:LYS:CG[2_765]	1.99	0.21
1:A:522:ASN:N	1:B:724:LYS:CD[3_855]	1.99	0.21
1:A:329:GLU:CG	1:A:982:ARG:NE[1_655]	2.01	0.19
1:A:289:GLU:CA	1:B:389:LYS:NZ[2_765]	2.02	0.18
1:A:575:TYR:CD1	1:B:898:LYS:C[3_845]	2.03	0.17
1:A:575:TYR:CZ	1:B:898:LYS:CA[3_845]	2.03	0.17
1:A:290:LEU:CD1	1:B:386:GLY:O[2_765]	2.03	0.17
1:A:953:LYS:O	1:B:574:VAL:CG2[1_655]	2.04	0.16
1:A:952:GLY:O	1:B:574:VAL:N[1_655]	2.04	0.16
1:A:950:ARG:NH1	1:B:579:GLU:OE2[1_655]	2.05	0.15
1:A:951:HIS:C	1:B:574:VAL:C[1_655]	2.05	0.15
1:A:952:GLY:CA	1:B:573:ASP:C[1_655]	2.08	0.12
1:A:388:GLU:OE1	1:A:507:THR:O[4_466]	2.09	0.11
1:A:949:LYS:CG	1:B:573:ASP:CG[1_655]	2.09	0.11
1:A:894:PRO:CB	1:B:575:TYR:OH[3_755]	2.09	0.11
1:A:491:LYS:NZ	1:B:288:GLU:OE1[3_855]	2.10	0.10
1:A:293:ASP:OD2	1:B:300:ARG:NH2[2_765]	2.10	0.10
1:A:953:LYS:CA	1:B:574:VAL:CA[1_655]	2.10	0.10
1:A:952:GLY:C	1:B:575:TYR:N[1_655]	2.12	0.08
1:A:894:PRO:C	1:B:575:TYR:CE1[3_755]	2.12	0.08
1:A:575:TYR:CD1	1:B:899:LYS:N[3_845]	2.13	0.07
1:A:952:GLY:N	1:B:574:VAL:CA[1_655]	2.14	0.06
1:A:521:GLU:CD	1:B:724:LYS:NZ[3_855]	2.14	0.06
1:A:953:LYS:N	1:B:574:VAL:C[1_655]	2.15	0.05
1:A:329:GLU:CG	1:A:982:ARG:CZ[1_655]	2.15	0.05
1:A:651:PRO:CB	1:B:899:LYS:CE[3_845]	2.15	0.05
1:A:289:GLU:OE1	1:B:389:LYS:CD[2_765]	2.16	0.04
1:A:329:GLU:CG	1:A:982:ARG:CD[1_655]	2.16	0.04
1:A:952:GLY:O	1:B:574:VAL:CB[1_655]	2.16	0.04
1:A:895:SER:CA	1:B:575:TYR:CZ[3_755]	2.16	0.04
1:A:293:ASP:OD1	1:B:300:ARG:CZ[2_765]	2.17	0.03
1:A:384:GLN:NE2	1:A:509:GLU:CD[4_466]	2.17	0.03
1:A:575:TYR:CZ	1:B:898:LYS:C[3_845]	2.18	0.02
1:A:895:SER:OG	1:B:575:TYR:CE1[3_755]	2.19	0.01
1:A:293:ASP:CG	1:B:300:ARG:CD[2_765]	2.19	0.01

## 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	744/847 (88%)	709 (95%)	31 (4%)	4 (0%)	29	67
1	B	745/847 (88%)	710 (95%)	31 (4%)	4 (0%)	29	67
All	All	1489/1694 (88%)	1419 (95%)	62 (4%)	8 (0%)	29	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1020	ASN
1	B	1020	ASN
1	A	497	ARG
1	A	508	ASN
1	B	497	ARG
1	B	508	ASN
1	A	440	CYS
1	B	440	CYS

### 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	698/773 (90%)	661 (95%)	37 (5%)	22	51
1	B	699/773 (90%)	656 (94%)	43 (6%)	18	46
All	All	1397/1546 (90%)	1317 (94%)	80 (6%)	20	49

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	255	LEU
1	A	259	LEU
1	A	260	LEU
1	A	271	ASP
1	A	304	ARG
1	A	356	LEU
1	A	428	ASN
1	A	458	GLU
1	A	463	LEU
1	A	497	ARG
1	A	498	LYS
1	A	508	ASN
1	A	510	TYR
1	A	511	LYS
1	A	519	LYS
1	A	529	LYS
1	A	544	LEU
1	A	547	ARG
1	A	575	TYR
1	A	576	ARG
1	A	615	TYR
1	A	640	LEU
1	A	676	ARG
1	A	679	LYS
1	A	680	GLU
1	A	722	ARG
1	A	724	LYS
1	A	808	VAL
1	A	821	LEU
1	A	831	LEU
1	A	860	GLN
1	A	885	ARG
1	A	919	LEU
1	A	930	PHE
1	A	968	THR
1	A	1040	VAL
1	B	214	GLN
1	B	235	LYS
1	B	255	LEU
1	B	258	LYS
1	B	259	LEU
1	B	260	LEU

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Mol	Chain	Res	Type
1	B	269	MET
1	B	356	LEU
1	B	389	LYS
1	B	421	LYS
1	B	428	ASN
1	B	456	LYS
1	B	463	LEU
1	B	498	LYS
1	B	504	LYS
1	B	509	GLU
1	B	510	TYR
1	B	511	LYS
1	B	519	LYS
1	B	529	LYS
1	B	544	LEU
1	B	547	ARG
1	B	575	TYR
1	B	576	ARG
1	B	615	TYR
1	B	640	LEU
1	B	676	ARG
1	B	679	LYS
1	B	680	GLU
1	B	722	ARG
1	B	724	LYS
1	B	767	ARG
1	B	808	VAL
1	B	821	LEU
1	B	831	LEU
1	B	860	GLN
1	B	885	ARG
1	B	899	LYS
1	B	919	LEU
1	B	930	PHE
1	B	968	THR
1	B	1036	LYS
1	B	1040	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN

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Mol	Chain	Res	Type
1	A	244	ASN
1	A	276	HIS
1	A	314	GLN
1	A	359	GLN
1	A	375	GLN
1	A	428	ASN
1	A	457	HIS
1	A	500	GLN
1	A	508	ASN
1	A	585	ASN
1	A	683	GLN
1	A	691	ASN
1	A	695	HIS
1	A	699	HIS
1	A	866	ASN
1	A	888	HIS
1	A	936	ASN
1	B	214	GLN
1	B	240	ASN
1	B	244	ASN
1	B	276	HIS
1	B	314	GLN
1	B	336	GLN
1	B	359	GLN
1	B	375	GLN
1	B	428	ASN
1	B	508	ASN
1	B	585	ASN
1	B	683	GLN
1	B	691	ASN
1	B	695	HIS
1	B	699	HIS
1	B	770	HIS
1	B	866	ASN
1	B	888	HIS
1	B	936	ASN

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	758/847 (89%)	0.26	37 (4%) 29 25	27, 27, 27, 27	0
1	B	759/847 (89%)	0.31	42 (5%) 25 21	27, 27, 27, 27	0
All	All	1517/1694 (89%)	0.28	79 (5%) 27 23	27, 27, 27, 27	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	969	GLY	5.9
1	B	498	LYS	5.8
1	B	549	THR	5.6
1	B	497	ARG	5.2
1	B	496	MET	5.0
1	B	493	LYS	4.3
1	A	811	LYS	4.3
1	B	501	ILE	4.2
1	B	495	PHE	4.1
1	B	439	GLN	4.0
1	B	462	PHE	4.0
1	B	438	GLY	3.9
1	A	944	ASN	3.9
1	A	968	THR	3.7
1	B	571	SER	3.6
1	B	653	PRO	3.5
1	A	810	THR	3.4
1	A	951	HIS	3.4
1	A	957	ASN	3.4
1	B	516	ILE	3.4
1	A	947	VAL	3.4
1	A	590	GLU	3.2
1	A	946	GLU	3.2
1	B	508	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	401	SER	3.2
1	A	272	GLU	3.1
1	B	543	SER	3.1
1	B	542	ILE	3.0
1	B	456	LYS	3.0
1	B	951	HIS	3.0
1	A	945	PRO	3.0
1	A	956	ILE	3.0
1	A	651	PRO	2.9
1	B	550	LEU	2.9
1	B	546	TYR	2.9
1	A	954	GLU	2.9
1	A	806	GLY	2.9
1	A	365	GLU	2.8
1	A	970	GLU	2.8
1	B	515	GLU	2.8
1	B	507	THR	2.7
1	B	548	SER	2.7
1	B	955	LEU	2.6
1	A	1044	ASN	2.6
1	A	949	LYS	2.6
1	A	943	GLY	2.6
1	A	488	TYR	2.5
1	A	1043	SER	2.5
1	A	935	THR	2.5
1	A	403	SER	2.5
1	A	722	ARG	2.5
1	B	492	GLU	2.4
1	B	499	VAL	2.4
1	A	950	ARG	2.4
1	B	420	LYS	2.4
1	B	398	ARG	2.4
1	A	404	ALA	2.4
1	A	361	GLU	2.3
1	B	1044	ASN	2.3
1	B	444	PHE	2.3
1	A	933	TYR	2.3
1	A	972	GLN	2.3
1	B	431	GLY	2.2
1	B	948	LEU	2.2
1	A	1023	PRO	2.2
1	A	586	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	404	ALA	2.2
1	B	288	GLU	2.2
1	B	547	ARG	2.2
1	B	539	ALA	2.2
1	A	948	LEU	2.2
1	B	506	ASP	2.1
1	A	906	GLU	2.1
1	B	474	ASN	2.1
1	B	950	ARG	2.1
1	B	490	LEU	2.1
1	A	473	SER	2.0
1	A	936	ASN	2.0
1	B	570	PRO	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.