



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:50 am GMT

PDB ID : 1JQO  
Title : Crystal structure of C4-form phosphoenolpyruvate carboxylase from maize  
Authors : Matsumura, H.; Kai, Y.  
Deposited on : 2001-08-07  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

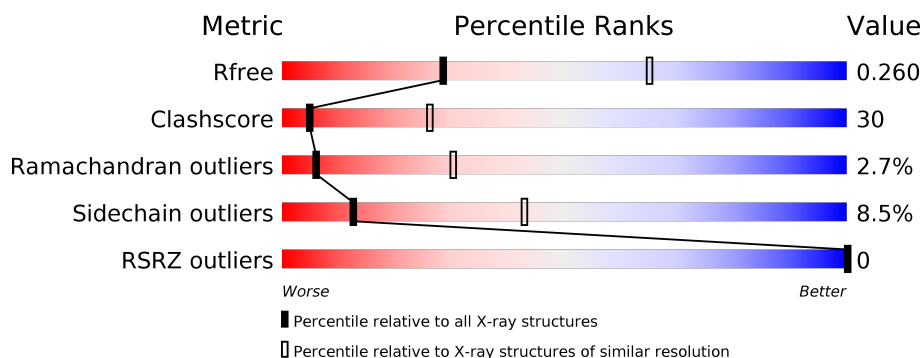
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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	970	
1	B	970	

## 2 Entry composition [i](#)

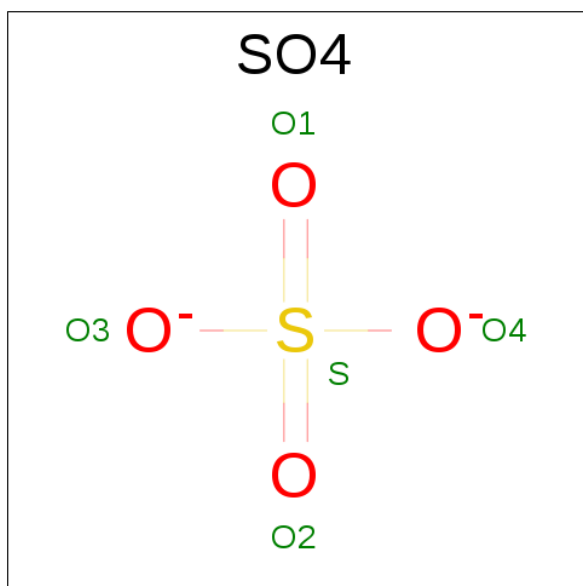
There are 2 unique types of molecules in this entry. The entry contains 14434 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 phosphoenolpyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7212	4584	1253	1345	30			
1	B	904	Total	C	N	O	S	0	0	0
			7212	4584	1253	1345	30			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

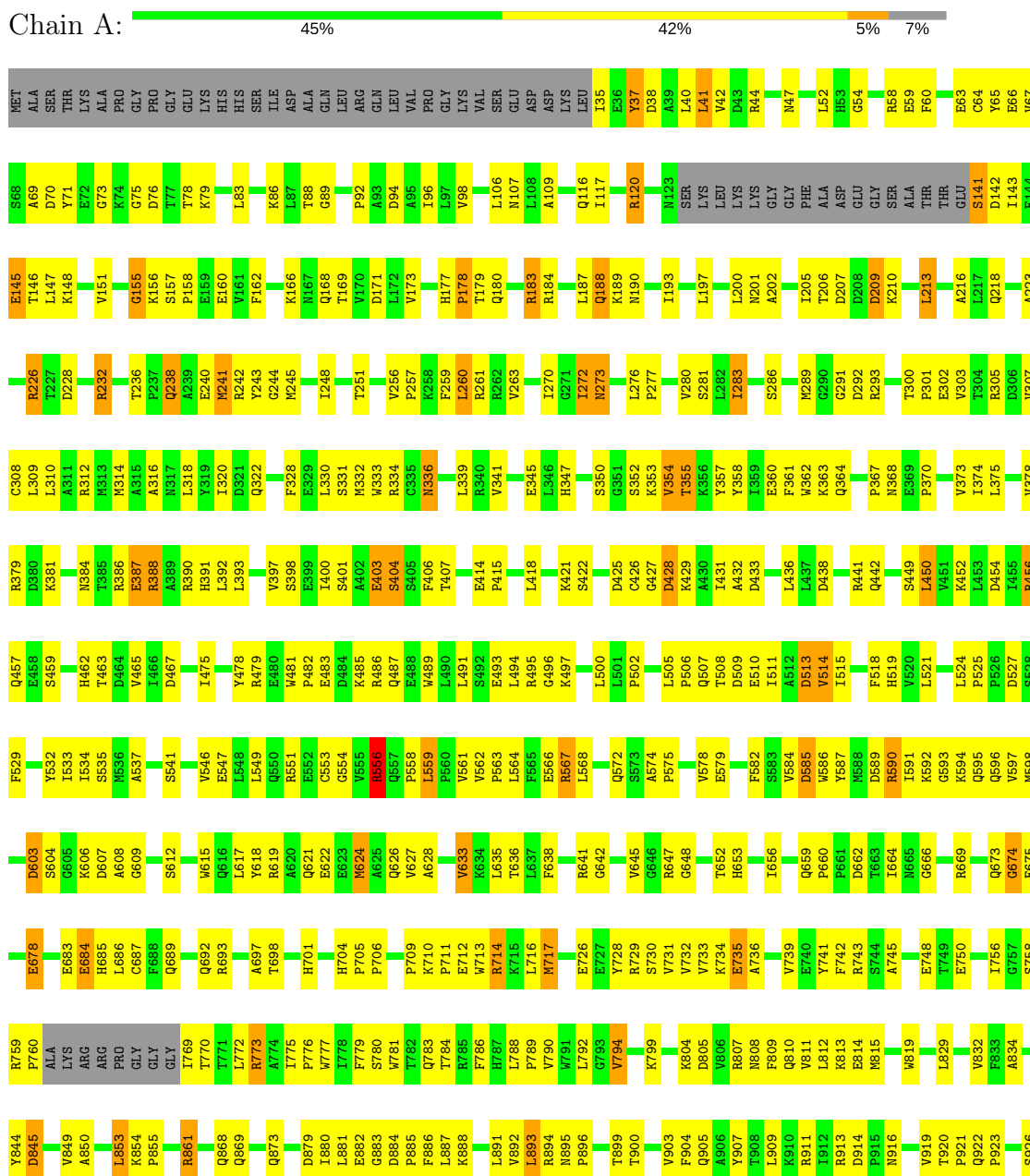


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots

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

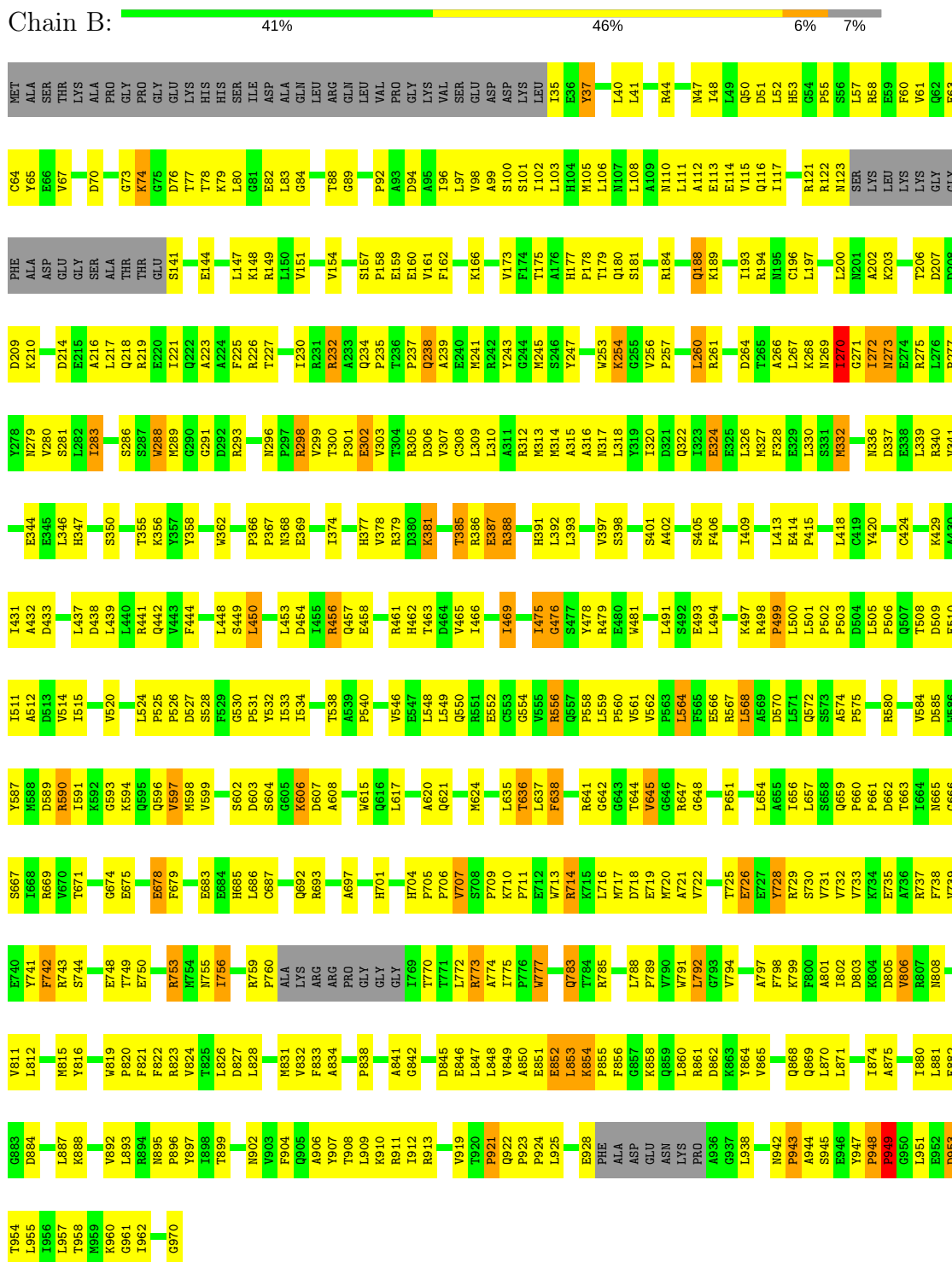
- Molecule 1: phosphoenolpyruvate carboxylase





### • Molecule 1: phosphoenolpyruvate carboxylase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.44Å 174.61Å 254.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.20 – 3.00 86.23 – 2.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (86.20-3.00) 79.6 (86.23-2.97)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.85 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.236 , 0.272 0.223 , 0.260	Depositor DCC
$R_{free}$ test set	2893 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.42	0/7365	0.61	0/9977
1	B	0.40	0/7365	0.59	0/9977
All	All	0.41	0/14730	0.60	0/19954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7212	0	7212	419	0
1	B	7212	0	7212	467	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
All	All	14434	0	14424	873	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 30.

All (873) 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:142:ASP:HA	1:A:692:GLN:HE21	1.19	1.06
1:B:505:LEU:HD12	1:B:506:PRO:HD2	1.30	1.05
1:B:502:PRO:HG2	1:B:505:LEU:HB2	1.40	1.02
1:A:179:THR:HG23	1:A:675:GLU:H	1.17	1.01
1:B:179:THR:HG23	1:B:675:GLU:H	1.27	0.98
1:A:505:LEU:HD12	1:A:506:PRO:HD2	1.48	0.96
1:A:683:GLU:HG3	1:A:684:GLU:H	1.33	0.93
1:B:50:GLN:HG3	1:B:55:PRO:HA	1.51	0.93
1:A:532:TYR:HB2	1:A:559:LEU:HD13	1.53	0.91
1:A:717:MET:HE2	1:A:717:MET:HA	1.52	0.91
1:A:769:ILE:HG23	1:A:772:LEU:HD12	1.54	0.88
1:A:853:LEU:H	1:A:853:LEU:HD23	1.38	0.87
1:A:162:PHE:HB2	1:A:272:ILE:HD13	1.54	0.86
1:B:683:GLU:H	1:B:686:LEU:HD12	1.40	0.86
1:A:587:TYR:CZ	1:A:591:ILE:HD11	2.11	0.85
1:B:562:VAL:HG23	1:B:597:VAL:HA	1.58	0.84
1:B:388:ARG:NH2	1:B:402:ALA:HA	1.93	0.84
1:A:788:LEU:HB3	1:A:789:PRO:HD3	1.59	0.83
1:B:188:GLN:HE22	1:B:189:LYS:NZ	1.74	0.83
1:A:179:THR:HG23	1:A:675:GLU:N	1.94	0.83
1:A:582:PHE:HE2	1:A:633:VAL:HG21	1.44	0.82
1:B:260:LEU:HD23	1:B:441:ARG:HD2	1.61	0.82
1:B:908:THR:HG23	1:B:951:LEU:HD22	1.62	0.82
1:B:568:LEU:HD12	1:B:608:ALA:HB2	1.61	0.81
1:A:238:GLN:H	1:A:238:GLN:NE2	1.76	0.81
1:B:848:LEU:HD22	1:B:913:ARG:HD2	1.61	0.81
1:B:103:LEU:HD13	1:B:961:GLY:HA2	1.63	0.81
1:B:101:SER:O	1:B:105:MET:HG3	1.81	0.80
1:A:510:GLU:O	1:A:514:VAL:HG12	1.81	0.79
1:B:184:ARG:HD3	1:B:243:TYR:HD1	1.47	0.79
1:B:414:GLU:HB3	1:B:415:PRO:HD3	1.61	0.79
1:A:507:GLN:HE22	1:A:515:ILE:HD12	1.48	0.79
1:B:574:ALA:HB3	1:B:575:PRO:HD3	1.64	0.79
1:B:568:LEU:HD22	1:B:572:GLN:HE21	1.48	0.79
1:B:273:ASN:H	1:B:273:ASN:HD22	1.31	0.79
1:A:145:GLU:HG2	1:A:146:THR:N	1.97	0.78
1:A:397:VAL:HG12	1:A:398:SER:H	1.46	0.78
1:B:833:PHE:HB3	1:B:868:GLN:HE21	1.48	0.78
1:B:564:LEU:HD23	1:B:598:MET:HG2	1.66	0.78
1:B:720:MET:HB3	1:B:797:ALA:HB1	1.65	0.78
1:A:582:PHE:CE2	1:A:633:VAL:HG21	2.19	0.77
1:B:96:ILE:HG21	1:B:938:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:ARG:O	1:B:865:VAL:HG23	1.86	0.76
1:B:465:VAL:O	1:B:469:ILE:HG23	1.86	0.76
1:B:854:LYS:NZ	1:B:854:LYS:HB2	2.01	0.75
1:B:397:VAL:HG12	1:B:398:SER:H	1.51	0.75
1:B:728:TYR:CD1	1:B:792:LEU:HD23	2.20	0.75
1:A:642:GLY:HA2	1:A:673:GLN:HG3	1.69	0.74
1:B:305:ARG:HA	1:B:524:LEU:HD11	1.67	0.74
1:B:854:LYS:N	1:B:855:PRO:HD2	2.01	0.74
1:A:743:ARG:HH21	1:A:769:ILE:HB	1.53	0.74
1:A:260:LEU:HD23	1:A:441:ARG:HD3	1.70	0.74
1:A:741:TYR:HB2	1:A:853:LEU:HD12	1.68	0.74
1:B:591:ILE:HG23	1:B:594:LYS:O	1.88	0.73
1:A:157:SER:HB3	1:A:160:GLU:HG3	1.69	0.73
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.69	0.73
1:B:925:LEU:H	1:B:925:LEU:HD12	1.53	0.73
1:B:491:LEU:HD21	1:B:584:VAL:HG11	1.70	0.73
1:A:205:ILE:CD1	1:A:210:LYS:HG3	2.18	0.73
1:B:293:ARG:HB3	1:B:293:ARG:NH1	2.03	0.73
1:B:465:VAL:HG22	1:B:511:ILE:HG23	1.69	0.73
1:A:236:THR:HB	1:A:238:GLN:NE2	2.03	0.73
1:A:595:GLN:NE2	1:A:596:GLN:H	1.87	0.73
1:A:743:ARG:HG2	1:A:743:ARG:HH11	1.55	0.72
1:B:888:LYS:O	1:B:892:VAL:HG23	1.90	0.72
1:B:337:ASP:O	1:B:341:VAL:HG23	1.88	0.72
1:B:188:GLN:NE2	1:B:189:LYS:HG3	2.04	0.72
1:A:309:LEU:HD21	1:A:392:LEU:HB3	1.72	0.71
1:A:731:VAL:HG11	1:A:792:LEU:HD21	1.71	0.71
1:A:750:GLU:HG3	1:A:955:LEU:HD21	1.73	0.71
1:B:388:ARG:O	1:B:392:LEU:HD13	1.89	0.71
1:A:868:GLN:OE1	1:A:880:ILE:HD11	1.91	0.71
1:A:502:PRO:HG2	1:A:505:LEU:HB2	1.71	0.71
1:B:206:THR:HG23	1:B:209:ASP:OD2	1.90	0.71
1:B:606:LYS:HD3	1:B:777:TRP:CD1	2.25	0.71
1:A:743:ARG:NH2	1:A:769:ILE:HB	2.06	0.70
1:B:188:GLN:HE22	1:B:189:LYS:HZ3	1.37	0.70
1:B:189:LYS:O	1:B:193:ILE:HG13	1.92	0.70
1:B:322:GLN:HG2	1:B:439:LEU:HD13	1.72	0.70
1:B:99:ALA:HB3	1:B:957:LEU:HD23	1.73	0.70
1:A:562:VAL:HG23	1:A:597:VAL:HA	1.73	0.70
1:A:508:THR:HB	1:A:511:ILE:CG1	2.23	0.69
1:B:247:TYR:OH	1:B:678:GLU:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ILE:HD13	1:A:283:ILE:H	1.57	0.69
1:B:173:VAL:HG22	1:B:286:SER:HB2	1.73	0.69
1:A:683:GLU:HG2	1:A:685:HIS:NE2	2.07	0.69
1:B:388:ARG:HH22	1:B:402:ALA:HA	1.56	0.69
1:B:273:ASN:H	1:B:273:ASN:ND2	1.90	0.69
1:A:35:ILE:N	1:A:116:GLN:OE1	2.26	0.69
1:B:64:CYS:HA	1:B:83:LEU:HD21	1.76	0.68
1:B:603:ASP:O	1:B:606:LYS:HB2	1.94	0.68
1:B:811:VAL:O	1:B:815:MET:HG3	1.93	0.68
1:B:909:LEU:O	1:B:913:ARG:HG3	1.94	0.68
1:A:574:ALA:HB3	1:A:575:PRO:HD3	1.76	0.67
1:A:937:GLY:HA2	1:A:940:LYS:HD2	1.76	0.67
1:B:568:LEU:HD22	1:B:572:GLN:NE2	2.08	0.67
1:B:718:ASP:O	1:B:721:ALA:HB3	1.95	0.67
1:B:731:VAL:HG11	1:B:792:LEU:HD21	1.76	0.67
1:B:912:ILE:HD13	1:B:947:TYR:CE1	2.30	0.67
1:A:893:LEU:HD22	1:A:893:LEU:O	1.95	0.67
1:B:505:LEU:HD12	1:B:506:PRO:CD	2.17	0.67
1:B:617:LEU:O	1:B:621:GLN:HG2	1.94	0.67
1:A:162:PHE:HB2	1:A:272:ILE:CD1	2.25	0.67
1:A:71:TYR:O	1:A:75:GLY:HA2	1.95	0.67
1:B:775:ILE:HG23	1:B:970:GLY:HA3	1.77	0.67
1:A:578:VAL:O	1:A:582:PHE:HD1	1.77	0.67
1:A:189:LYS:O	1:A:193:ILE:HG13	1.95	0.67
1:A:142:ASP:HA	1:A:692:GLN:NE2	2.02	0.66
1:A:966:MET:O	1:A:967:GLN:HB2	1.95	0.66
1:A:595:GLN:HE21	1:A:596:GLN:H	1.42	0.66
1:A:683:GLU:HG3	1:A:684:GLU:N	2.09	0.66
1:A:922:GLN:HB3	1:A:923:PRO:HD2	1.77	0.66
1:B:954:THR:O	1:B:958:THR:HG23	1.96	0.66
1:A:347:HIS:CE1	1:A:367:PRO:HD3	2.31	0.66
1:B:660:PRO:HG2	1:B:663:THR:HG21	1.78	0.66
1:A:582:PHE:CE2	1:A:633:VAL:HG11	2.31	0.65
1:B:728:TYR:O	1:B:731:VAL:HG12	1.95	0.65
1:A:363:LYS:NZ	1:B:239:ALA:HB2	2.11	0.65
1:B:241:MET:HG2	1:B:307:VAL:HG12	1.78	0.65
1:A:205:ILE:HD12	1:A:210:LYS:HG3	1.77	0.65
1:B:238:GLN:NE2	1:B:238:GLN:H	1.94	0.65
1:A:162:PHE:CE2	1:A:166:LYS:HD2	2.32	0.65
1:A:534:ILE:HD11	1:A:561:VAL:HG11	1.79	0.65
1:B:493:GLU:OE1	1:B:500:LEU:HD22	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:TYR:HB2	1:A:559:LEU:CD1	2.26	0.65
1:A:883:GLY:O	1:A:885:PRO:HD3	1.97	0.65
1:B:853:LEU:CD2	1:B:853:LEU:H	2.10	0.64
1:A:158:PRO:O	1:A:272:ILE:HD11	1.96	0.64
1:A:52:LEU:HD22	1:A:226:ARG:HH21	1.62	0.64
1:B:456:ARG:HG2	1:B:533:ILE:HB	1.80	0.64
1:A:309:LEU:HD23	1:A:393:LEU:HG	1.79	0.64
1:A:732:VAL:HG23	1:A:733:VAL:HG23	1.78	0.64
1:A:656:ILE:HD12	1:A:697:ALA:HB3	1.80	0.64
1:B:534:ILE:HD11	1:B:561:VAL:CG1	2.28	0.64
1:B:853:LEU:HD23	1:B:853:LEU:H	1.61	0.64
1:A:508:THR:HB	1:A:511:ILE:HG12	1.80	0.64
1:A:107:ASN:HD21	1:A:190:ASN:HD21	1.45	0.63
1:B:37:TYR:HA	1:B:40:LEU:HB3	1.79	0.63
1:A:617:LEU:O	1:A:621:GLN:HG2	1.99	0.63
1:B:742:PHE:CZ	1:B:748:GLU:HG3	2.34	0.63
1:B:731:VAL:CG1	1:B:792:LEU:HD21	2.28	0.63
1:B:943:PRO:HG2	1:B:944:ALA:H	1.63	0.63
1:B:728:TYR:HD1	1:B:792:LEU:HD23	1.64	0.63
1:B:151:VAL:HG11	1:B:158:PRO:HG3	1.79	0.63
1:A:35:ILE:N	1:A:116:GLN:HE22	1.97	0.62
1:A:809:PHE:CE2	1:A:813:LYS:HD2	2.35	0.62
1:A:726:GLU:O	1:A:730:SER:HB3	2.00	0.62
1:A:641:ARG:HD3	1:A:648:GLY:O	1.99	0.62
1:B:469:ILE:HD13	1:B:500:LEU:HG	1.79	0.62
1:A:500:LEU:O	1:A:502:PRO:HD3	1.98	0.62
1:B:654:LEU:O	1:B:657:LEU:HB3	1.99	0.62
1:A:188:GLN:HE22	1:A:189:LYS:NZ	1.97	0.62
1:B:237:PRO:HB2	1:B:303:VAL:HG11	1.82	0.62
1:A:151:VAL:O	1:A:155:GLY:HA2	2.00	0.61
1:A:236:THR:HB	1:A:238:GLN:HE22	1.63	0.61
1:B:683:GLU:N	1:B:686:LEU:HD12	2.13	0.61
1:A:148:LYS:HG3	1:A:270:ILE:HD11	1.82	0.61
1:B:644:THR:HG23	1:B:970:GLY:O	2.00	0.61
1:A:714:ARG:HH11	1:A:714:ARG:HG3	1.66	0.61
1:A:574:ALA:O	1:A:578:VAL:HG23	2.00	0.61
1:A:117:ILE:HD11	1:A:886:PHE:HE2	1.65	0.61
1:B:52:LEU:HD13	1:B:226:ARG:NH1	2.15	0.61
1:A:591:ILE:HG23	1:A:594:LYS:O	2.01	0.61
1:B:388:ARG:HH21	1:B:401:SER:C	2.04	0.61
1:B:726:GLU:O	1:B:730:SER:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:GLN:HB3	1:B:923:PRO:HD2	1.83	0.61
1:B:512:ALA:HA	1:B:515:ILE:HG22	1.82	0.60
1:B:538:THR:HG22	1:B:567:ARG:HH22	1.66	0.60
1:B:179:THR:CG2	1:B:675:GLU:H	2.09	0.60
1:A:336:ASN:HB2	1:A:422:SER:HA	1.82	0.60
1:B:743:ARG:HE	1:B:749:THR:HG23	1.66	0.60
1:B:805:ASP:OD1	1:B:806:VAL:N	2.34	0.60
1:A:595:GLN:HE21	1:A:596:GLN:N	2.00	0.60
1:B:288:TRP:CD1	1:B:454:ASP:HB2	2.36	0.60
1:B:948:PRO:HB2	1:B:949:PRO:HD2	1.84	0.60
1:A:362:TRP:HE1	1:A:363:LYS:HZ3	1.48	0.60
1:A:67:VAL:HG13	1:A:79:LYS:HD2	1.84	0.60
1:A:293:ARG:HG2	1:A:456:ARG:O	2.02	0.60
1:B:188:GLN:HE22	1:B:189:LYS:HZ2	1.48	0.60
1:A:226:ARG:HG3	1:A:226:ARG:HH11	1.65	0.60
1:A:709:PRO:HG2	1:A:714:ARG:NH1	2.16	0.60
1:A:147:LEU:O	1:A:151:VAL:HG23	2.02	0.60
1:A:595:GLN:O	1:A:635:LEU:HA	2.02	0.60
1:A:659:GLN:O	1:A:701:HIS:HE1	1.83	0.60
1:A:794:VAL:HG21	1:A:829:LEU:HD21	1.83	0.60
1:B:298:ARG:NH2	1:B:760:PRO:HB3	2.17	0.60
1:B:635:LEU:HD21	1:B:637:LEU:CD2	2.32	0.60
1:A:790:VAL:HG11	1:A:832:VAL:HG21	1.84	0.59
1:A:783:GLN:HE22	1:A:959:MET:HA	1.66	0.59
1:A:63:GLU:OE2	1:A:86:LYS:HE3	2.01	0.59
1:B:831:MET:O	1:B:834:ALA:HB3	2.01	0.59
1:A:148:LYS:HG3	1:A:270:ILE:CD1	2.32	0.59
1:A:628:ALA:HB1	1:A:633:VAL:HG22	1.84	0.59
1:B:254:LYS:O	1:B:257:PRO:HD2	2.03	0.59
1:B:298:ARG:HH21	1:B:760:PRO:HB3	1.68	0.59
1:B:683:GLU:HB2	1:B:686:LEU:HG	1.84	0.59
1:A:283:ILE:N	1:A:283:ILE:HD13	2.17	0.59
1:A:731:VAL:CG1	1:A:792:LEU:HD21	2.32	0.59
1:A:609:GLY:HA2	1:A:728:TYR:CD1	2.38	0.59
1:A:948:PRO:HG2	1:A:951:LEU:HD12	1.85	0.59
1:B:340:ARG:O	1:B:344:GLU:HB2	2.03	0.59
1:B:272:ILE:H	1:B:272:ILE:HD12	1.67	0.59
1:B:868:GLN:NE2	1:B:880:ILE:HD11	2.18	0.59
1:B:99:ALA:CB	1:B:957:LEU:HD23	2.33	0.59
1:B:347:HIS:CD2	1:B:367:PRO:HD3	2.38	0.59
1:B:47:ASN:O	1:B:51:ASP:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD22	1:B:356:LYS:HB3	1.85	0.59
1:B:300:THR:HB	1:B:301:PRO:HD2	1.85	0.59
1:B:313:MET:O	1:B:317:ASN:HB2	2.03	0.59
1:B:645:VAL:HG21	1:B:832:VAL:HG22	1.85	0.59
1:B:70:ASP:O	1:B:74:LYS:HB2	2.03	0.59
1:B:788:LEU:HB3	1:B:789:PRO:HD3	1.83	0.58
1:B:254:LYS:N	1:B:254:LYS:HD2	2.17	0.58
1:B:293:ARG:HB3	1:B:293:ARG:HH11	1.68	0.58
1:A:244:GLY:HA3	1:A:289:MET:HE1	1.85	0.58
1:B:241:MET:HG2	1:B:307:VAL:CG1	2.34	0.58
1:A:270:ILE:HG22	1:A:270:ILE:O	2.02	0.58
1:A:850:ALA:HB3	1:A:853:LEU:HD21	1.86	0.58
1:A:888:LYS:O	1:A:892:VAL:HG23	2.03	0.58
1:B:147:LEU:HD23	1:B:161:VAL:HG11	1.86	0.58
1:B:111:LEU:HD22	1:B:194:ARG:HG3	1.85	0.58
1:B:88:THR:HG22	1:B:911:ARG:HD2	1.85	0.58
1:B:925:LEU:N	1:B:925:LEU:HD12	2.19	0.58
1:B:635:LEU:HD23	1:B:635:LEU:C	2.25	0.58
1:A:300:THR:HB	1:A:301:PRO:HD2	1.85	0.58
1:B:641:ARG:HD3	1:B:648:GLY:O	2.04	0.58
1:B:706:PRO:HB3	1:B:820:PRO:HG2	1.85	0.58
1:B:845:ASP:HA	1:B:849:VAL:CG2	2.34	0.58
1:A:456:ARG:HG3	1:A:533:ILE:HB	1.86	0.57
1:A:534:ILE:HD11	1:A:561:VAL:CG1	2.34	0.57
1:A:907:TYR:O	1:A:911:ARG:HG3	2.03	0.57
1:B:273:ASN:N	1:B:273:ASN:HD22	1.92	0.57
1:A:884:ASP:OD1	1:A:887:LEU:HB2	2.04	0.57
1:B:308:CYS:SG	1:B:528:SER:HB2	2.44	0.57
1:B:845:ASP:C	1:B:847:LEU:H	2.07	0.57
1:B:850:ALA:HB3	1:B:853:LEU:CD2	2.34	0.57
1:B:53:HIS:HD2	1:B:97:LEU:HD13	1.68	0.57
1:A:728:TYR:CE2	1:A:732:VAL:HG21	2.39	0.57
1:A:716:LEU:HD23	1:A:815:MET:HE1	1.86	0.57
1:B:709:PRO:HB3	1:B:819:TRP:CZ2	2.40	0.57
1:A:184:ARG:HD3	1:A:243:TYR:HD1	1.69	0.57
1:B:462:HIS:CE1	1:B:532:TYR:HE2	2.23	0.57
1:A:291:GLY:HA3	1:A:454:ASP:O	2.04	0.57
1:B:312:ARG:NH2	1:B:527:ASP:OD2	2.37	0.57
1:A:293:ARG:HG3	1:A:457:GLN:OE1	2.05	0.57
1:A:551:ARG:NH1	1:A:558:PRO:HG3	2.19	0.57
1:B:635:LEU:HD21	1:B:637:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:THR:HB	1:A:693:ARG:HG2	1.86	0.57
1:B:567:ARG:NH2	1:B:570:ASP:OD1	2.38	0.57
1:B:709:PRO:HB3	1:B:819:TRP:CE2	2.39	0.57
1:A:213:LEU:O	1:A:216:ALA:HB3	2.05	0.57
1:B:41:LEU:HG	1:B:108:LEU:HD22	1.87	0.57
1:B:50:GLN:HB2	1:B:58:ARG:HB2	1.86	0.57
1:B:301:PRO:O	1:B:520:VAL:HG21	2.05	0.57
1:B:912:ILE:HD13	1:B:947:TYR:CD1	2.40	0.57
1:A:92:PRO:O	1:A:96:ILE:HG12	2.06	0.56
1:B:178:PRO:HG2	1:B:775:ILE:HD12	1.87	0.56
1:B:238:GLN:HE21	1:B:238:GLN:H	1.51	0.56
1:B:44:ARG:HH11	1:B:44:ARG:HG2	1.69	0.56
1:B:854:LYS:HB2	1:B:854:LYS:HZ3	1.69	0.56
1:A:432:ALA:O	1:A:436:LEU:HB3	2.04	0.56
1:A:505:LEU:HD12	1:A:506:PRO:CD	2.31	0.56
1:A:59:GLU:O	1:A:63:GLU:HG3	2.06	0.56
1:A:509:ASP:O	1:A:513:ASP:HB2	2.05	0.56
1:A:807:ARG:HH11	1:A:807:ARG:HG3	1.71	0.56
1:B:392:LEU:HD12	1:B:392:LEU:N	2.21	0.56
1:A:177:HIS:O	1:A:179:THR:N	2.38	0.56
1:A:94:ASP:O	1:A:98:VAL:HG23	2.06	0.56
1:B:449:SER:O	1:B:450:LEU:CB	2.52	0.56
1:A:180:GLN:O	1:A:756:ILE:HG23	2.05	0.56
1:B:508:THR:HG22	1:B:509:ASP:N	2.20	0.56
1:B:858:LYS:O	1:B:858:LYS:HD3	2.05	0.56
1:A:467:ASP:CG	1:A:479:ARG:HG3	2.26	0.56
1:B:463:THR:HB	1:B:479:ARG:HH21	1.70	0.56
1:B:232:ARG:N	1:B:232:ARG:HD2	2.21	0.56
1:B:816:TYR:CD2	1:B:875:ALA:HA	2.41	0.56
1:A:151:VAL:HG13	1:A:156:LYS:O	2.06	0.56
1:A:355:THR:HG22	1:A:357:TYR:HE2	1.71	0.56
1:B:159:GLU:N	1:B:159:GLU:OE2	2.39	0.56
1:B:717:MET:CE	1:B:717:MET:HA	2.36	0.56
1:B:310:LEU:O	1:B:314:MET:HG3	2.06	0.55
1:B:534:ILE:HD11	1:B:561:VAL:HG11	1.87	0.55
1:B:65:TYR:CE1	1:B:896:PRO:HG2	2.41	0.55
1:A:438:ASP:O	1:A:442:GLN:HG3	2.07	0.55
1:A:524:LEU:HD12	1:A:529:PHE:HZ	1.71	0.55
1:A:459:SER:HB2	1:A:534:ILE:CG2	2.35	0.55
1:A:89:GLY:HA3	1:A:922:GLN:HG3	1.87	0.55
1:B:854:LYS:N	1:B:855:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:LEU:O	1:B:874:ILE:HG12	2.06	0.55
1:A:273:ASN:N	1:A:273:ASN:HD22	2.03	0.55
1:B:339:LEU:HG	1:B:374:ILE:CD1	2.37	0.55
1:B:441:ARG:HH11	1:B:441:ARG:HG3	1.72	0.55
1:B:819:TRP:CE3	1:B:822:PHE:HB2	2.41	0.55
1:B:567:ARG:CZ	1:B:570:ASP:OD2	2.55	0.55
1:B:615:TRP:CZ2	1:B:714:ARG:HD2	2.42	0.55
1:A:584:VAL:HG12	1:A:587:TYR:H	1.71	0.55
1:B:602:SER:HB3	1:B:774:ALA:CB	2.37	0.55
1:B:919:VAL:O	1:B:921:PRO:HD3	2.07	0.55
1:A:653:HIS:CD2	1:A:653:HIS:H	2.24	0.55
1:A:805:ASP:OD1	1:A:807:ARG:N	2.39	0.55
1:B:339:LEU:HG	1:B:374:ILE:HD11	1.88	0.55
1:B:824:VAL:O	1:B:828:LEU:HG	2.07	0.55
1:A:728:TYR:HE2	1:A:732:VAL:HG21	1.71	0.55
1:B:732:VAL:HG23	1:B:733:VAL:HG23	1.89	0.54
1:B:469:ILE:CD1	1:B:500:LEU:HG	2.37	0.54
1:B:253:TRP:HD1	1:B:254:LYS:HE3	1.71	0.54
1:B:861:ARG:HG2	1:B:861:ARG:HH11	1.72	0.54
1:A:341:VAL:HG12	1:A:345:GLU:OE1	2.08	0.54
1:A:664:ILE:HG21	1:A:698:THR:HG23	1.90	0.54
1:A:415:PRO:O	1:A:418:LEU:HB3	2.08	0.54
1:A:742:PHE:HD2	1:A:781:TRP:CZ2	2.25	0.54
1:B:149:ARG:O	1:B:154:VAL:HG23	2.07	0.54
1:B:615:TRP:CH2	1:B:714:ARG:HD2	2.42	0.54
1:B:720:MET:HG2	1:B:797:ALA:O	2.08	0.54
1:A:388:ARG:O	1:A:392:LEU:HD13	2.06	0.54
1:B:267:LEU:HA	1:B:270:ILE:HD13	1.90	0.54
1:B:339:LEU:HD12	1:B:418:LEU:HG	1.89	0.54
1:B:275:ARG:HD2	1:B:433:ASP:OD2	2.07	0.54
1:B:462:HIS:HE1	1:B:532:TYR:HE2	1.56	0.54
1:B:466:ILE:HD11	1:B:549:LEU:HG	1.89	0.54
1:A:374:ILE:O	1:A:378:VAL:HG23	2.08	0.54
1:A:483:GLU:OE2	1:A:541:SER:HB3	2.07	0.54
1:A:582:PHE:CD2	1:A:633:VAL:HG11	2.43	0.54
1:B:508:THR:HB	1:B:511:ILE:HG12	1.89	0.54
1:B:283:ILE:HD13	1:B:283:ILE:H	1.72	0.53
1:B:743:ARG:NE	1:B:749:THR:HG23	2.23	0.53
1:A:310:LEU:O	1:A:314:MET:HG3	2.09	0.53
1:A:845:ASP:HA	1:A:849:VAL:HG23	1.89	0.53
1:A:844:TYR:HE2	1:A:905:GLN:HE21	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HD11	1:B:957:LEU:HD13	1.90	0.53
1:A:277:PRO:HG2	1:A:280:VAL:CG2	2.39	0.53
1:A:363:LYS:HZ2	1:B:239:ALA:HB2	1.71	0.53
1:B:74:LYS:HB3	1:B:76:ASP:OD1	2.08	0.53
1:A:177:HIS:O	1:A:179:THR:HG22	2.09	0.53
1:B:683:GLU:HB3	1:B:685:HIS:CD2	2.43	0.53
1:B:845:ASP:HA	1:B:849:VAL:HG23	1.89	0.53
1:A:456:ARG:HD2	1:A:535:SER:OG	2.07	0.53
1:B:366:PRO:HG2	1:B:369:GLU:HG3	1.90	0.53
1:A:188:GLN:HE22	1:A:189:LYS:HZ2	1.56	0.53
1:B:508:THR:HB	1:B:511:ILE:H	1.73	0.53
1:A:462:HIS:HE2	1:A:532:TYR:HH	1.57	0.53
1:A:566:GLU:HG2	1:A:603:ASP:HB2	1.90	0.53
1:A:759:ARG:HD3	1:A:773:ARG:NH2	2.23	0.53
1:A:854:LYS:N	1:A:855:PRO:HD2	2.23	0.53
1:B:774:ALA:O	1:B:777:TRP:HB3	2.09	0.53
1:A:582:PHE:HE2	1:A:633:VAL:HG11	1.73	0.53
1:B:820:PRO:O	1:B:824:VAL:HG23	2.09	0.53
1:A:710:LYS:HB3	1:A:711:PRO:HD2	1.90	0.52
1:B:88:THR:HB	1:B:919:VAL:HG11	1.91	0.52
1:B:893:LEU:HD13	1:B:893:LEU:O	2.08	0.52
1:B:261:ARG:O	1:B:264:ASP:HB2	2.09	0.52
1:B:494:LEU:HD23	1:B:548:LEU:HD12	1.90	0.52
1:A:35:ILE:N	1:A:116:GLN:NE2	2.58	0.52
1:B:247:TYR:CE2	1:B:678:GLU:HA	2.44	0.52
1:B:823:ARG:HG2	1:B:827:ASP:OD2	2.09	0.52
1:A:37:TYR:H	1:A:37:TYR:HD1	1.52	0.52
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.91	0.52
1:B:177:HIS:C	1:B:179:THR:H	2.13	0.52
1:A:66:GLU:O	1:A:69:ALA:HB3	2.10	0.52
1:A:742:PHE:CZ	1:A:748:GLU:HG3	2.45	0.52
1:A:714:ARG:NH1	1:A:714:ARG:HG3	2.25	0.52
1:A:894:ARG:NH1	1:A:894:ARG:HG3	2.25	0.52
1:B:564:LEU:CD2	1:B:598:MET:HG2	2.36	0.52
1:B:567:ARG:HB2	1:B:570:ASP:OD2	2.09	0.52
1:B:773:ARG:HG2	1:B:773:ARG:HH11	1.75	0.52
1:A:809:PHE:HE2	1:A:813:LYS:HD2	1.75	0.51
1:A:812:LEU:HD23	1:A:815:MET:CE	2.40	0.51
1:B:157:SER:O	1:B:161:VAL:HG23	2.10	0.51
1:A:156:LYS:HD2	1:A:160:GLU:OE1	2.11	0.51
1:A:511:ILE:O	1:A:515:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:HA	1:B:272:ILE:O	2.10	0.51
1:B:388:ARG:NH2	1:B:402:ALA:CA	2.71	0.51
1:A:316:ALA:O	1:A:320:ILE:HG13	2.09	0.51
1:A:853:LEU:N	1:A:853:LEU:HD23	2.17	0.51
1:B:121:ARG:C	1:B:123:ASN:H	2.13	0.51
1:B:35:ILE:HG12	1:B:35:ILE:O	2.10	0.51
1:B:401:SER:OG	1:B:402:ALA:N	2.44	0.51
1:B:50:GLN:HG3	1:B:55:PRO:CA	2.33	0.51
1:B:216:ALA:HA	1:B:219:ARG:HG2	1.92	0.51
1:A:948:PRO:HB2	1:A:949:PRO:HD2	1.92	0.51
1:B:141:SER:O	1:B:692:GLN:HG2	2.10	0.51
1:A:241:MET:O	1:A:245:MET:HB2	2.10	0.51
1:A:452:LYS:HE3	1:A:527:ASP:O	2.09	0.51
1:A:209:ASP:O	1:A:213:LEU:HD12	2.11	0.51
1:A:618:TYR:CD1	1:A:660:PRO:HD3	2.46	0.51
1:A:647:ARG:NE	1:A:775:ILE:HD13	2.25	0.51
1:A:60:PHE:CE1	1:A:86:LYS:HD2	2.45	0.51
1:B:214:ASP:O	1:B:218:GLN:HG3	2.11	0.51
1:A:339:LEU:CD2	1:A:370:PRO:HB3	2.41	0.51
1:B:234:GLN:HB2	1:B:755:ASN:HD22	1.76	0.51
1:B:266:ALA:O	1:B:270:ILE:HG23	2.11	0.51
1:B:273:ASN:N	1:B:273:ASN:ND2	2.56	0.51
1:B:461:ARG:HG2	1:B:461:ARG:HH11	1.75	0.51
1:B:638:PHE:HA	1:B:669:ARG:HB2	1.93	0.51
1:A:292:ASP:CG	1:A:456:ARG:HH21	2.13	0.51
1:A:414:GLU:HB3	1:A:415:PRO:HD3	1.93	0.51
1:A:635:LEU:HD23	1:A:635:LEU:C	2.32	0.51
1:B:728:TYR:CE1	1:B:792:LEU:HD23	2.46	0.51
1:A:141:SER:HB2	1:A:145:GLU:OE2	2.11	0.50
1:A:38:ASP:O	1:A:42:VAL:HG23	2.11	0.50
1:B:598:MET:HA	1:B:638:PHE:HB3	1.93	0.50
1:B:884:ASP:OD1	1:B:887:LEU:HD13	2.11	0.50
1:A:244:GLY:HA3	1:A:289:MET:CE	2.41	0.50
1:A:743:ARG:NH1	1:A:748:GLU:OE2	2.44	0.50
1:B:141:SER:HA	1:B:693:ARG:CZ	2.42	0.50
1:B:449:SER:O	1:B:450:LEU:HB3	2.10	0.50
1:B:538:THR:CG2	1:B:567:ARG:HH22	2.25	0.50
1:B:816:TYR:CE2	1:B:875:ALA:HA	2.46	0.50
1:A:245:MET:CE	1:A:248:ILE:HG13	2.41	0.50
1:A:489:TRP:O	1:A:493:GLU:HG2	2.12	0.50
1:B:100:SER:O	1:B:103:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:OE2	1:B:148:LYS:HE3	2.11	0.50
1:A:236:THR:O	1:A:240:GLU:HG3	2.12	0.50
1:A:384:ASN:O	1:A:388:ARG:HB2	2.11	0.50
1:A:391:HIS:HB2	1:A:398:SER:HB2	1.93	0.50
1:A:534:ILE:HG22	1:A:537:ALA:HB2	1.94	0.50
1:A:334:ARG:NH1	1:B:226:ARG:NH2	2.60	0.50
1:B:750:GLU:HG3	1:B:955:LEU:HD21	1.93	0.50
1:A:65:TYR:CE1	1:A:896:PRO:HG2	2.47	0.50
1:A:428:ASP:CG	1:B:226:ARG:HG2	2.32	0.50
1:B:856:PHE:O	1:B:860:LEU:HD23	2.12	0.50
1:B:881:LEU:HD13	1:B:887:LEU:HB3	1.93	0.50
1:A:276:LEU:HD23	1:A:277:PRO:O	2.12	0.50
1:A:567:ARG:HH21	1:A:607:ASP:HB3	1.77	0.50
1:B:180:GLN:O	1:B:180:GLN:HG3	2.11	0.50
1:B:309:LEU:HB3	1:B:393:LEU:HD21	1.93	0.50
1:B:783:GLN:HE22	1:B:962:ILE:HB	1.75	0.50
1:A:242:ARG:NH2	1:A:310:LEU:HD22	2.26	0.50
1:A:717:MET:CE	1:A:717:MET:HA	2.35	0.50
1:A:956:ILE:HD12	1:A:956:ILE:H	1.76	0.50
1:B:607:ASP:OD2	1:B:608:ALA:N	2.45	0.50
1:B:731:VAL:HG13	1:B:732:VAL:HG13	1.94	0.50
1:A:547:GLU:CD	1:A:590:ARG:HH21	2.16	0.50
1:B:636:THR:HB	1:B:667:SER:OG	2.11	0.50
1:A:564:LEU:HD13	1:A:598:MET:SD	2.51	0.49
1:B:716:LEU:HG	1:B:720:MET:HE2	1.93	0.49
1:A:339:LEU:HG	1:A:374:ILE:HD11	1.94	0.49
1:B:785:ARG:NH2	1:B:899:THR:HA	2.27	0.49
1:A:141:SER:O	1:A:692:GLN:HG2	2.12	0.49
1:A:775:ILE:N	1:A:776:PRO:HD2	2.27	0.49
1:B:568:LEU:HD12	1:B:608:ALA:CB	2.39	0.49
1:A:494:LEU:HD13	1:A:586:TRP:CZ3	2.47	0.49
1:B:842:GLY:O	1:B:845:ASP:HB2	2.12	0.49
1:A:334:ARG:HH11	1:B:226:ARG:NH2	2.10	0.49
1:A:312:ARG:HG2	1:A:449:SER:HB3	1.94	0.49
1:A:595:GLN:NE2	1:A:596:GLN:N	2.59	0.49
1:B:293:ARG:HH12	1:B:299:VAL:HG12	1.77	0.49
1:B:391:HIS:HB2	1:B:398:SER:HB2	1.95	0.49
1:B:247:TYR:HE2	1:B:678:GLU:HA	1.76	0.49
1:A:781:TRP:HA	1:A:784:THR:HG22	1.95	0.49
1:B:753:ARG:HH11	1:B:753:ARG:HG2	1.77	0.49
1:A:353:LYS:HB3	1:A:364:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PRO:O	1:A:373:VAL:HB	2.12	0.49
1:A:401:SER:OG	1:A:404:SER:HB3	2.12	0.49
1:B:546:VAL:O	1:B:550:GLN:HB2	2.13	0.49
1:A:622:GLU:OE2	1:A:714:ARG:NH2	2.46	0.49
1:B:298:ARG:HG2	1:B:298:ARG:HH11	1.78	0.49
1:A:427:GLY:O	1:A:429:LYS:N	2.45	0.49
1:A:533:ILE:HG12	1:A:562:VAL:HG13	1.95	0.49
1:A:534:ILE:CG2	1:A:537:ALA:HB2	2.43	0.48
1:B:44:ARG:NH1	1:B:44:ARG:HG2	2.27	0.48
1:B:735:GLU:OE2	1:B:737:ARG:HB3	2.11	0.48
1:B:884:ASP:OD1	1:B:887:LEU:HD22	2.13	0.48
1:A:76:ASP:OD1	1:A:79:LYS:HG2	2.13	0.48
1:B:200:LEU:HD11	1:B:210:LYS:HG3	1.95	0.48
1:B:826:LEU:HD22	1:B:871:LEU:CD1	2.43	0.48
1:A:582:PHE:HE2	1:A:633:VAL:CG2	2.23	0.48
1:A:619:ARG:HH11	1:A:619:ARG:HG2	1.79	0.48
1:B:253:TRP:CD1	1:B:254:LYS:HE3	2.49	0.48
1:B:725:THR:O	1:B:728:TYR:HB3	2.13	0.48
1:A:487:GLN:O	1:A:491:LEU:HB2	2.13	0.48
1:A:861:ARG:HG2	1:A:861:ARG:HH11	1.77	0.48
1:A:183:ARG:HB2	2:A:971:SO4:O2	2.13	0.48
1:B:709:PRO:HA	1:B:713:TRP:HE3	1.78	0.48
1:A:330:LEU:HD12	1:A:375:LEU:HD11	1.95	0.48
1:A:845:ASP:HA	1:A:849:VAL:CG2	2.43	0.48
1:B:293:ARG:HG2	1:B:456:ARG:O	2.12	0.48
1:A:331:SER:O	1:B:227:THR:HG23	2.13	0.48
1:A:894:ARG:HH11	1:A:894:ARG:HG3	1.77	0.48
1:B:743:ARG:HH11	1:B:743:ARG:HG2	1.78	0.48
1:B:803:ASP:O	1:B:805:ASP:N	2.46	0.48
1:A:355:THR:HG22	1:A:357:TYR:CE2	2.48	0.48
1:A:390:ARG:CZ	1:A:390:ARG:HB3	2.42	0.48
1:A:421:LYS:HE2	1:A:425:ASP:OD1	2.14	0.48
1:A:462:HIS:ND1	1:A:546:VAL:HG22	2.28	0.48
1:B:44:ARG:O	1:B:48:ILE:HG13	2.14	0.48
1:B:92:PRO:O	1:B:96:ILE:HG12	2.14	0.48
1:A:47:ASN:N	1:A:47:ASN:HD22	2.11	0.48
1:A:683:GLU:HB3	1:A:686:LEU:HG	1.95	0.48
1:A:850:ALA:HB3	1:A:853:LEU:CD2	2.44	0.48
1:A:853:LEU:CD2	1:A:853:LEU:H	2.18	0.48
1:B:777:TRP:HE3	1:B:777:TRP:HA	1.79	0.48
1:A:273:ASN:H	1:A:273:ASN:ND2	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:CA	1:A:692:GLN:HE21	2.09	0.47
1:A:779:PHE:HD1	1:A:969:THR:O	1.97	0.47
1:A:854:LYS:HB3	1:A:855:PRO:CD	2.44	0.47
1:B:177:HIS:HB3	1:B:775:ILE:HD11	1.95	0.47
1:B:845:ASP:OD1	1:B:849:VAL:HG21	2.13	0.47
1:B:847:LEU:HD13	1:B:906:ALA:HB1	1.96	0.47
1:A:184:ARG:HD3	1:A:243:TYR:CD1	2.49	0.47
1:A:508:THR:HG22	1:A:510:GLU:H	1.78	0.47
1:A:593:GLY:O	1:A:633:VAL:HB	2.14	0.47
1:A:638:PHE:CD1	1:A:669:ARG:HB3	2.48	0.47
1:B:853:LEU:HD23	1:B:853:LEU:N	2.29	0.47
1:A:261:ARG:NH2	1:A:433:ASP:O	2.46	0.47
1:B:178:PRO:CG	1:B:775:ILE:HD12	2.44	0.47
1:B:409:ILE:HG12	1:B:448:LEU:HD22	1.96	0.47
1:B:57:LEU:O	1:B:61:VAL:HG23	2.14	0.47
1:A:456:ARG:CG	1:A:533:ILE:HB	2.45	0.47
1:A:947:TYR:HB3	1:A:948:PRO:HD2	1.97	0.47
1:B:110:ASN:O	1:B:114:GLU:HG3	2.14	0.47
1:B:461:ARG:HG2	1:B:461:ARG:NH1	2.28	0.47
1:A:578:VAL:O	1:A:582:PHE:CD1	2.63	0.47
1:A:899:THR:O	1:A:903:VAL:HG23	2.14	0.47
1:A:948:PRO:CG	1:A:951:LEU:HD12	2.45	0.47
1:B:162:PHE:CE2	1:B:166:LYS:HD2	2.50	0.47
1:B:355:THR:O	1:B:358:TYR:HB2	2.15	0.47
1:B:550:GLN:OE1	1:B:559:LEU:N	2.47	0.47
1:B:89:GLY:O	1:B:922:GLN:HB2	2.15	0.47
1:B:925:LEU:H	1:B:925:LEU:CD1	2.24	0.47
1:A:891:LEU:O	1:A:895:ASN:ND2	2.48	0.47
1:B:184:ARG:HD3	1:B:243:TYR:CD1	2.38	0.47
1:B:234:GLN:CG	1:B:235:PRO:HD2	2.44	0.47
1:B:732:VAL:HA	1:B:738:PHE:CD2	2.50	0.47
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.78	0.47
1:A:482:PRO:HG2	1:A:485:LYS:HB2	1.97	0.47
1:B:777:TRP:HA	1:B:777:TRP:CE3	2.49	0.47
1:B:816:TYR:CG	1:B:816:TYR:O	2.67	0.47
1:B:858:LYS:O	1:B:862:ASP:OD1	2.32	0.47
1:B:230:ILE:HD12	1:B:953:ASP:OD2	2.14	0.47
1:A:179:THR:O	1:A:675:GLU:HB2	2.15	0.47
1:A:273:ASN:N	1:A:273:ASN:ND2	2.63	0.47
1:A:305:ARG:O	1:A:309:LEU:HB2	2.15	0.47
1:A:428:ASP:OD1	1:B:226:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLU:HB2	1:A:780:SER:OG	2.15	0.47
1:A:809:PHE:CD2	1:A:813:LYS:HD2	2.49	0.47
1:A:717:MET:HG3	1:A:819:TRP:HZ3	1.80	0.47
1:A:283:ILE:CD1	1:A:283:ILE:N	2.78	0.47
1:B:279:ASN:HA	1:B:444:PHE:CD2	2.49	0.47
1:B:819:TRP:CZ2	1:B:821:PHE:HD2	2.33	0.47
1:A:568:LEU:HD22	1:A:608:ALA:HB2	1.97	0.46
1:B:60:PHE:HE2	1:B:98:VAL:HG11	1.80	0.46
1:A:69:ALA:O	1:A:73:GLY:N	2.44	0.46
1:B:241:MET:O	1:B:245:MET:HB2	2.15	0.46
1:B:296:ASN:ND2	1:B:759:ARG:HA	2.30	0.46
1:B:748:GLU:OE2	1:B:749:THR:N	2.49	0.46
1:B:851:GLU:HA	1:B:854:LYS:HZ3	1.80	0.46
1:A:592:LYS:HG2	1:A:592:LYS:O	2.16	0.46
1:A:579:GLU:HB2	1:A:627:VAL:HG11	1.97	0.46
1:A:656:ILE:HD12	1:A:697:ALA:CB	2.45	0.46
1:B:254:LYS:H	1:B:254:LYS:HD2	1.80	0.46
1:B:441:ARG:NH1	1:B:441:ARG:HG3	2.30	0.46
1:B:508:THR:CB	1:B:511:ILE:HG12	2.46	0.46
1:B:773:ARG:NH1	1:B:773:ARG:HG2	2.31	0.46
1:A:384:ASN:O	1:A:388:ARG:CB	2.64	0.46
1:A:729:ARG:O	1:A:733:VAL:HB	2.15	0.46
1:B:397:VAL:HG12	1:B:398:SER:N	2.26	0.46
1:B:50:GLN:O	1:B:50:GLN:HG2	2.16	0.46
1:B:864:TYR:HD2	1:B:865:VAL:N	2.13	0.46
1:A:173:VAL:HB	1:A:286:SER:HB2	1.96	0.46
1:A:238:GLN:H	1:A:238:GLN:CD	2.18	0.46
1:A:653:HIS:CD2	1:A:653:HIS:N	2.84	0.46
1:B:316:ALA:O	1:B:320:ILE:HG13	2.16	0.46
1:B:659:GLN:O	1:B:701:HIS:HE1	1.98	0.46
1:A:226:ARG:NH1	1:A:226:ARG:HG3	2.30	0.46
1:A:465:VAL:CG2	1:A:514:VAL:HG11	2.45	0.46
1:A:179:THR:CG2	1:A:675:GLU:H	2.07	0.46
1:A:730:SER:HA	1:A:734:LYS:HB2	1.98	0.46
1:B:420:TYR:CD1	1:B:432:ALA:HB1	2.50	0.46
1:A:386:ARG:HD2	1:A:387:GLU:OE2	2.16	0.46
1:A:759:ARG:HD3	1:A:773:ARG:HH22	1.81	0.46
1:B:117:ILE:O	1:B:121:ARG:HB2	2.16	0.46
1:B:178:PRO:HA	1:B:756:ILE:HG22	1.97	0.46
1:A:143:ILE:H	1:A:692:GLN:NE2	2.14	0.46
1:A:228:ASP:OD2	1:A:232:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLU:O	1:B:117:ILE:HG12	2.16	0.46
1:B:47:ASN:HD22	1:B:58:ARG:HH12	1.62	0.46
1:B:744:SER:OG	1:B:849:VAL:HA	2.16	0.46
1:A:735:GLU:OE2	1:A:736:ALA:N	2.49	0.46
1:B:217:LEU:HD23	1:B:217:LEU:O	2.15	0.46
1:B:864:TYR:CD2	1:B:865:VAL:N	2.84	0.46
1:A:683:GLU:H	1:A:686:LEU:HD12	1.81	0.45
1:A:743:ARG:HG2	1:A:743:ARG:NH1	2.27	0.45
1:B:709:PRO:HA	1:B:713:TRP:CE3	2.51	0.45
1:B:803:ASP:C	1:B:805:ASP:N	2.68	0.45
1:B:899:THR:O	1:B:902:ASN:N	2.46	0.45
1:B:53:HIS:CD2	1:B:97:LEU:HD13	2.51	0.45
1:A:333:TRP:HA	1:A:370:PRO:HD2	1.98	0.45
1:A:572:GLN:C	1:A:574:ALA:H	2.19	0.45
1:B:76:ASP:OD2	1:B:79:LYS:HG2	2.17	0.45
1:B:845:ASP:C	1:B:847:LEU:N	2.70	0.45
1:A:201:ASN:N	1:A:201:ASN:HD22	2.13	0.45
1:A:202:ALA:HB3	1:A:205:ILE:HG23	1.98	0.45
1:A:357:TYR:H	1:A:357:TYR:HD2	1.64	0.45
1:A:769:ILE:CG2	1:A:772:LEU:HD12	2.38	0.45
1:A:745:ALA:HB2	1:A:849:VAL:CG2	2.47	0.45
1:B:753:ARG:HG2	1:B:753:ARG:NH1	2.31	0.45
1:B:854:LYS:HZ2	1:B:854:LYS:HB2	1.77	0.45
1:B:948:PRO:HG2	1:B:951:LEU:HD12	1.98	0.45
1:A:37:TYR:N	1:A:37:TYR:CD1	2.76	0.45
1:B:178:PRO:HD2	1:B:775:ILE:HD12	1.99	0.45
1:B:392:LEU:CD1	1:B:392:LEU:N	2.80	0.45
1:B:438:ASP:O	1:B:442:GLN:HG3	2.17	0.45
1:B:494:LEU:HD23	1:B:548:LEU:CD1	2.47	0.45
1:B:742:PHE:CE2	1:B:748:GLU:HB2	2.51	0.45
1:B:94:ASP:O	1:B:98:VAL:HG23	2.17	0.45
1:A:758:SER:O	1:A:760:PRO:HD3	2.17	0.45
1:A:808:ASN:HA	1:A:811:VAL:HG23	1.98	0.45
1:B:448:LEU:N	1:B:448:LEU:HD22	2.32	0.45
1:B:525:PRO:HA	1:B:526:PRO:HD3	1.82	0.45
1:B:454:ASP:OD1	1:B:531:PRO:HD2	2.17	0.45
1:A:169:THR:HG23	1:A:281:SER:O	2.17	0.45
1:B:103:LEU:HD13	1:B:961:GLY:CA	2.42	0.45
1:B:144:GLU:HG3	1:B:266:ALA:HA	1.97	0.45
1:B:508:THR:C	1:B:510:GLU:N	2.70	0.45
1:A:157:SER:HB3	1:A:160:GLU:CG	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLN:HG2	1:A:673:GLN:H	1.57	0.45
1:A:713:TRP:N	1:A:713:TRP:CD1	2.84	0.45
1:A:645:VAL:HG21	1:A:832:VAL:CG2	2.47	0.45
1:B:788:LEU:HD12	1:B:791:TRP:CZ2	2.52	0.45
1:A:63:GLU:O	1:A:66:GLU:N	2.50	0.45
1:B:141:SER:HA	1:B:693:ARG:NH1	2.31	0.45
1:A:318:LEU:HD12	1:A:450:LEU:HD21	1.98	0.44
1:A:813:LYS:NZ	1:A:813:LYS:HB3	2.32	0.44
1:B:413:LEU:O	1:B:414:GLU:C	2.54	0.44
1:B:660:PRO:HA	1:B:661:PRO:HD3	1.83	0.44
1:A:564:LEU:CD1	1:A:598:MET:HG2	2.47	0.44
1:B:719:GLU:O	1:B:722:VAL:HG22	2.17	0.44
1:B:106:LEU:HD13	1:B:897:TYR:HB3	1.99	0.44
1:B:88:THR:CG2	1:B:911:ARG:HD2	2.47	0.44
1:A:957:LEU:O	1:A:960:LYS:HB2	2.18	0.44
1:A:966:MET:O	1:A:967:GLN:CB	2.63	0.44
1:B:502:PRO:HA	1:B:503:PRO:HD3	1.82	0.44
1:A:162:PHE:CD2	1:A:166:LYS:HD2	2.53	0.44
1:A:54:GLY:N	1:A:927:LYS:HE3	2.33	0.44
1:A:88:THR:O	1:A:919:VAL:HG11	2.17	0.44
1:B:508:THR:HG22	1:B:509:ASP:H	1.82	0.44
1:B:705:PRO:HA	1:B:706:PRO:HD3	1.88	0.44
1:B:738:PHE:O	1:B:741:TYR:N	2.51	0.44
1:A:145:GLU:HG2	1:A:146:THR:H	1.79	0.44
1:A:459:SER:HB2	1:A:534:ILE:HG22	1.99	0.44
1:B:202:ALA:O	1:B:203:LYS:HD3	2.17	0.44
1:B:386:ARG:HG3	1:B:386:ARG:HH11	1.82	0.44
1:B:656:ILE:HD12	1:B:697:ALA:HB3	1.98	0.44
1:A:384:ASN:HB3	1:A:400:ILE:HG21	2.00	0.44
1:A:549:LEU:O	1:A:553:CYS:HB2	2.17	0.44
1:B:293:ARG:HG3	1:B:457:GLN:NE2	2.33	0.44
1:B:587:TYR:CE2	1:B:591:ILE:HD11	2.52	0.44
1:A:178:PRO:HA	1:A:756:ILE:HG22	2.00	0.44
1:A:809:PHE:O	1:A:813:LYS:HG3	2.17	0.44
1:B:102:ILE:O	1:B:106:LEU:HB2	2.17	0.44
1:B:385:THR:OG1	1:B:405:SER:HB2	2.17	0.44
1:A:223:ALA:HA	1:B:431:ILE:HD11	1.99	0.44
1:B:508:THR:C	1:B:510:GLU:H	2.20	0.44
1:B:63:GLU:O	1:B:67:VAL:HG23	2.18	0.44
1:B:716:LEU:HD11	1:B:801:ALA:HB1	2.00	0.44
1:A:659:GLN:O	1:A:701:HIS:CE1	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:OE2	1:B:379:ARG:HD2	2.18	0.44
1:B:533:ILE:HG12	1:B:562:VAL:HG13	2.00	0.44
1:A:585:ASP:O	1:A:589:ASP:HB2	2.17	0.44
1:B:469:ILE:O	1:B:469:ILE:HD12	2.18	0.44
1:B:855:PRO:HG2	1:B:856:PHE:H	1.82	0.44
1:B:942:ASN:OD1	1:B:945:SER:HB2	2.18	0.44
1:A:525:PRO:HB2	1:A:527:ASP:OD2	2.18	0.43
1:A:893:LEU:HD22	1:A:893:LEU:C	2.38	0.43
1:B:157:SER:HB3	1:B:160:GLU:CG	2.48	0.43
1:B:293:ARG:CB	1:B:293:ARG:HH11	2.29	0.43
1:B:381:LYS:HG2	1:B:406:PHE:CE2	2.52	0.43
1:B:500:LEU:N	1:B:552:GLU:OE1	2.51	0.43
1:B:230:ILE:HA	1:B:960:LYS:HE3	1.99	0.43
1:A:403:GLU:HG2	1:A:403:GLU:H	1.33	0.43
1:A:743:ARG:NH1	1:A:743:ARG:CG	2.81	0.43
1:B:309:LEU:HA	1:B:309:LEU:HD12	1.89	0.43
1:A:242:ARG:HD2	1:B:362:TRP:CD1	2.54	0.43
1:B:456:ARG:CG	1:B:533:ILE:HB	2.47	0.43
1:B:823:ARG:HG2	1:B:823:ARG:HH11	1.82	0.43
1:A:360:GLU:O	1:A:361:PHE:HB2	2.18	0.43
1:A:619:ARG:O	1:A:622:GLU:HB3	2.18	0.43
1:A:742:PHE:HD2	1:A:781:TRP:HZ2	1.64	0.43
1:B:346:LEU:HD23	1:B:377:HIS:HB2	2.00	0.43
1:B:710:LYS:O	1:B:711:PRO:C	2.55	0.43
1:A:508:THR:HB	1:A:511:ILE:CB	2.47	0.43
1:A:673:GLN:O	1:A:674:GLY:C	2.56	0.43
1:A:743:ARG:HH11	1:A:743:ARG:CG	2.24	0.43
1:A:739:VAL:HG21	1:A:770:THR:HG22	1.99	0.43
1:A:226:ARG:HB3	1:B:332:MET:HG3	2.00	0.43
1:B:501:LEU:HD21	1:B:515:ILE:HD11	2.00	0.43
1:B:591:ILE:HD13	1:B:591:ILE:HA	1.83	0.43
1:B:638:PHE:CD2	1:B:669:ARG:HD3	2.53	0.43
1:B:638:PHE:HE1	1:B:671:THR:HG23	1.82	0.43
1:B:845:ASP:O	1:B:847:LEU:N	2.52	0.43
1:A:37:TYR:HD2	1:A:197:LEU:HD22	1.82	0.43
1:A:562:VAL:HA	1:A:563:PRO:HD3	1.80	0.43
1:A:429:LYS:O	1:A:432:ALA:HB3	2.19	0.43
1:A:704:HIS:N	1:A:705:PRO:HD3	2.33	0.43
1:A:909:LEU:O	1:A:913:ARG:HG3	2.18	0.43
1:B:37:TYR:HB2	1:B:112:ALA:HB1	2.00	0.43
1:B:475:ILE:HG13	1:B:481:TRP:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ARG:HA	1:B:732:VAL:HG22	2.01	0.43
1:A:41:LEU:CD1	1:A:197:LEU:HD11	2.49	0.43
1:A:518:PHE:O	1:A:521:LEU:HB2	2.19	0.43
1:A:494:LEU:HD13	1:A:586:TRP:CE3	2.53	0.43
1:A:607:ASP:OD2	1:A:607:ASP:N	2.51	0.43
1:A:920:THR:HA	1:A:921:PRO:HD3	1.79	0.43
1:A:942:ASN:OD1	1:A:945:SER:HB2	2.18	0.43
1:B:53:HIS:HE1	1:B:226:ARG:HH12	1.67	0.43
1:B:798:PHE:O	1:B:799:LYS:C	2.57	0.43
1:A:259:PHE:O	1:A:263:VAL:HG23	2.19	0.43
1:A:804:LYS:HE2	1:A:808:ASN:HD21	1.84	0.43
1:A:717:MET:HG3	1:A:819:TRP:CZ3	2.54	0.43
1:B:324:GLU:O	1:B:327:MET:HB2	2.18	0.43
1:B:838:PRO:O	1:B:841:ALA:HB3	2.19	0.43
1:B:910:LYS:C	1:B:912:ILE:N	2.72	0.43
1:A:171:ASP:OD1	1:A:173:VAL:HG12	2.18	0.43
1:A:510:GLU:OE1	1:A:510:GLU:N	2.52	0.43
1:A:784:THR:HG23	1:A:786:PHE:HB2	2.01	0.43
1:B:462:HIS:O	1:B:466:ILE:HG12	2.19	0.43
1:A:467:ASP:OD1	1:A:479:ARG:HG3	2.19	0.43
1:A:783:GLN:NE2	1:A:959:MET:HA	2.32	0.43
1:B:409:ILE:HG12	1:B:448:LEU:CD2	2.49	0.43
1:B:50:GLN:HB2	1:B:58:ARG:CB	2.49	0.43
1:B:532:TYR:CD2	1:B:546:VAL:HG11	2.54	0.43
1:B:910:LYS:C	1:B:912:ILE:H	2.21	0.43
1:B:642:GLY:N	1:B:647:ARG:O	2.50	0.42
1:B:748:GLU:OE1	1:B:772:LEU:HD11	2.19	0.42
1:B:65:TYR:HE1	1:B:896:PRO:HG2	1.83	0.42
1:A:142:ASP:HB3	1:A:145:GLU:HB3	2.02	0.42
1:A:811:VAL:O	1:A:814:GLU:N	2.52	0.42
1:A:868:GLN:CD	1:A:880:ILE:HD11	2.39	0.42
1:B:50:GLN:HB2	1:B:58:ARG:HD2	2.01	0.42
1:B:812:LEU:HD23	1:B:815:MET:HE2	1.99	0.42
1:A:350:SER:C	1:A:352:SER:H	2.23	0.42
1:A:362:TRP:CG	1:A:363:LYS:N	2.87	0.42
1:A:368:ASN:O	1:A:370:PRO:HD3	2.19	0.42
1:A:70:ASP:HB2	1:A:79:LYS:HG3	2.00	0.42
1:A:83:LEU:HD21	1:A:900:THR:HG23	2.00	0.42
1:B:475:ILE:HD12	1:B:476:GLY:H	1.83	0.42
1:B:478:TYR:O	1:B:481:TRP:N	2.45	0.42
1:B:596:GLN:OE1	1:B:638:PHE:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:ARG:HH22	1:B:899:THR:HA	1.84	0.42
1:B:783:GLN:HE22	1:B:962:ILE:HD12	1.85	0.42
1:A:273:ASN:H	1:A:273:ASN:HD22	1.66	0.42
1:B:540:PRO:HG2	1:B:580:ARG:HG2	2.01	0.42
1:B:707:VAL:HG23	1:B:820:PRO:HD3	2.01	0.42
1:A:41:LEU:HD11	1:A:197:LEU:HD11	2.02	0.42
1:A:478:TYR:CZ	1:A:486:ARG:HD3	2.55	0.42
1:A:431:ILE:HD13	1:B:223:ALA:HA	2.02	0.42
1:B:366:PRO:HB2	1:B:368:ASN:HD22	1.84	0.42
1:B:392:LEU:CD1	1:B:392:LEU:H	2.32	0.42
1:B:510:GLU:O	1:B:514:VAL:HG12	2.20	0.42
1:B:564:LEU:HD23	1:B:598:MET:CG	2.44	0.42
1:B:73:GLY:O	1:B:74:LYS:HD3	2.20	0.42
1:A:564:LEU:HD13	1:A:598:MET:CG	2.49	0.42
1:B:217:LEU:O	1:B:221:ILE:HG13	2.19	0.42
1:A:116:GLN:HG2	1:A:120:ARG:CZ	2.50	0.42
1:A:358:TYR:CE2	1:A:379:ARG:CZ	3.03	0.42
1:A:47:ASN:N	1:A:47:ASN:ND2	2.68	0.42
1:A:508:THR:O	1:A:509:ASP:C	2.55	0.42
1:A:626:GLN:C	1:A:628:ALA:N	2.71	0.42
1:A:363:LYS:HZ1	1:B:239:ALA:HB2	1.82	0.42
1:B:277:PRO:HG2	1:B:280:VAL:HG21	2.02	0.42
1:B:305:ARG:O	1:B:309:LEU:HB2	2.18	0.42
1:B:84:GLY:HA3	1:B:907:TYR:CZ	2.55	0.42
1:B:850:ALA:HB3	1:B:853:LEU:HD21	2.01	0.42
1:B:853:LEU:C	1:B:855:PRO:HD2	2.40	0.42
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.82	0.42
1:A:307:VAL:HG23	1:A:308:CYS:N	2.35	0.42
1:A:63:GLU:O	1:A:64:CYS:C	2.58	0.42
1:B:560:PRO:HA	1:B:590:ARG:NH2	2.35	0.42
1:B:792:LEU:HD12	1:B:792:LEU:HA	1.82	0.42
1:B:805:ASP:HB3	1:B:808:ASN:ND2	2.35	0.42
1:B:895:ASN:O	1:B:897:TYR:N	2.53	0.42
1:A:353:LYS:HB2	1:A:364:GLN:H	1.84	0.42
1:A:310:LEU:HA	1:A:393:LEU:HD11	2.01	0.42
1:A:481:TRP:HZ3	1:A:489:TRP:CB	2.33	0.42
1:A:507:GLN:HA	1:A:507:GLN:OE1	2.20	0.42
1:A:556:ARG:CD	1:A:556:ARG:H	2.32	0.42
1:B:106:LEU:HD13	1:B:897:TYR:CB	2.49	0.42
1:B:461:ARG:HE	1:B:510:GLU:HB3	1.85	0.42
1:A:792:LEU:HD12	1:A:792:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:ASP:OD1	1:A:916:ASN:OD1	2.38	0.41
1:B:271:GLY:O	1:B:272:ILE:C	2.59	0.41
1:B:453:LEU:O	1:B:530:GLY:N	2.31	0.41
1:B:591:ILE:HG22	1:B:593:GLY:N	2.34	0.41
1:A:381:LYS:HG2	1:A:406:PHE:CE1	2.55	0.41
1:A:390:ARG:NH1	1:A:390:ARG:HB3	2.35	0.41
1:A:772:LEU:O	1:A:773:ARG:O	2.38	0.41
1:A:809:PHE:HZ	1:A:873:GLN:HB3	1.86	0.41
1:B:151:VAL:CG1	1:B:158:PRO:HG3	2.50	0.41
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.80	0.41
1:A:157:SER:O	1:A:160:GLU:N	2.53	0.41
1:A:463:THR:HG22	1:A:479:ARG:NH1	2.35	0.41
1:B:277:PRO:HG2	1:B:280:VAL:CG2	2.50	0.41
1:B:291:GLY:HA3	1:B:454:ASP:O	2.20	0.41
1:B:387:GLU:HA	1:B:387:GLU:OE1	2.19	0.41
1:B:558:PRO:O	1:B:559:LEU:C	2.58	0.41
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.95	0.41
1:A:429:LYS:O	1:A:432:ALA:N	2.51	0.41
1:A:705:PRO:HA	1:A:706:PRO:HD3	1.88	0.41
1:A:891:LEU:C	1:A:895:ASN:HD22	2.23	0.41
1:B:313:MET:HE3	1:B:393:LEU:HD12	2.02	0.41
1:B:374:ILE:O	1:B:378:VAL:HG23	2.20	0.41
1:B:315:ALA:HB2	1:B:450:LEU:HB2	2.02	0.41
1:B:568:LEU:O	1:B:572:GLN:HG3	2.20	0.41
1:B:77:THR:O	1:B:80:LEU:HB2	2.20	0.41
1:A:547:GLU:OE1	1:A:547:GLU:HA	2.20	0.41
1:B:47:ASN:HD22	1:B:58:ARG:NH1	2.18	0.41
1:B:599:VAL:HG12	1:B:617:LEU:HD21	2.03	0.41
1:A:210:LYS:HA	1:A:213:LEU:HD12	2.03	0.41
1:A:926:SER:C	1:A:928:GLU:H	2.24	0.41
1:B:147:LEU:HD23	1:B:161:VAL:CG1	2.50	0.41
1:B:283:ILE:O	1:B:283:ILE:HD13	2.20	0.41
1:B:44:ARG:CZ	1:B:214:ASP:OD1	2.69	0.41
1:B:651:PRO:HG2	1:B:654:LEU:HD12	2.03	0.41
1:B:742:PHE:C	1:B:742:PHE:CD2	2.94	0.41
1:B:773:ARG:HD2	1:B:773:ARG:HA	1.90	0.41
1:A:106:LEU:O	1:A:109:ALA:HB3	2.19	0.41
1:A:116:GLN:HG2	1:A:120:ARG:NE	2.36	0.41
1:A:44:ARG:HD2	1:A:218:GLN:HG2	2.02	0.41
1:A:500:LEU:HD12	1:A:500:LEU:N	2.35	0.41
1:A:919:VAL:CG1	1:A:920:THR:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ILE:HG22	1:B:593:GLY:H	1.86	0.41
1:B:783:GLN:NE2	1:B:962:ILE:HB	2.36	0.41
1:B:498:ARG:HA	1:B:499:PRO:HD3	1.94	0.41
1:B:512:ALA:HA	1:B:515:ILE:CG2	2.51	0.41
1:B:234:GLN:CB	1:B:755:ASN:HD22	2.33	0.41
1:B:76:ASP:C	1:B:78:THR:H	2.23	0.41
1:B:880:ILE:C	1:B:882:GLU:N	2.74	0.41
1:A:162:PHE:O	1:A:166:LYS:HG3	2.20	0.41
1:A:303:VAL:O	1:A:307:VAL:HG13	2.21	0.41
1:A:40:LEU:HD12	1:A:44:ARG:NH1	2.36	0.41
1:A:515:ILE:HG22	1:A:519:HIS:CD2	2.56	0.41
1:A:562:VAL:HG23	1:A:596:GLN:O	2.21	0.41
1:A:201:ASN:N	1:A:201:ASN:ND2	2.69	0.41
1:A:812:LEU:HD23	1:A:815:MET:HE3	2.02	0.41
1:A:54:GLY:CA	1:A:927:LYS:HE3	2.51	0.41
1:B:225:PHE:C	1:B:227:THR:H	2.24	0.41
1:B:293:ARG:NH1	1:B:299:VAL:O	2.54	0.41
1:B:566:GLU:O	1:B:604:SER:HA	2.21	0.41
1:A:171:ASP:O	1:A:669:ARG:HA	2.20	0.40
1:B:599:VAL:HG11	1:B:617:LEU:HD23	2.01	0.40
1:B:735:GLU:HG3	1:B:738:PHE:H	1.85	0.40
1:B:923:PRO:HA	1:B:924:PRO:HD3	1.99	0.40
1:A:157:SER:CB	1:A:160:GLU:OE2	2.69	0.40
1:A:35:ILE:N	1:A:116:GLN:CD	2.75	0.40
1:A:518:PHE:HA	1:A:521:LEU:HD12	2.03	0.40
1:A:52:LEU:HD22	1:A:226:ARG:NH2	2.33	0.40
1:A:578:VAL:HG21	1:A:624:MET:SD	2.61	0.40
1:A:834:ALA:HB2	1:A:881:LEU:HG	2.03	0.40
1:A:879:ASP:O	1:A:882:GLU:HB2	2.21	0.40
1:B:111:LEU:O	1:B:115:VAL:HG23	2.22	0.40
1:B:302:GLU:O	1:B:305:ARG:HG2	2.21	0.40
1:B:326:LEU:HG	1:B:326:LEU:O	2.21	0.40
1:B:424:CYS:SG	1:B:429:LYS:HG2	2.62	0.40
1:B:566:GLU:HG2	1:B:603:ASP:HB2	2.03	0.40
1:B:617:LEU:O	1:B:620:ALA:HB3	2.20	0.40
1:B:799:LYS:O	1:B:802:ILE:HB	2.20	0.40
1:B:175:THR:HG22	1:B:288:TRP:HB2	2.03	0.40
1:B:253:TRP:CD2	1:B:318:LEU:HD13	2.57	0.40
1:B:716:LEU:HG	1:B:720:MET:CE	2.51	0.40
1:A:143:ILE:O	1:A:147:LEU:HG	2.22	0.40
1:A:168:GLN:HG3	1:A:666:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:TRP:O	1:A:618:TYR:HB3	2.21	0.40
1:A:179:THR:C	1:A:675:GLU:HB2	2.42	0.40
1:A:187:LEU:HD22	1:A:678:GLU:HG3	2.03	0.40
1:A:777:TRP:CZ2	1:A:789:PRO:HG3	2.57	0.40
1:B:196:CYS:O	1:B:200:LEU:HB2	2.21	0.40
1:B:178:PRO:O	1:B:756:ILE:HG21	2.21	0.40
1:B:812:LEU:HD23	1:B:815:MET:CE	2.52	0.40
1:A:491:LEU:O	1:A:495:ARG:HG3	2.22	0.40
1:B:283:ILE:HD13	1:B:283:ILE:N	2.37	0.40
1:B:704:HIS:N	1:B:705:PRO:HD3	2.36	0.40
1:B:948:PRO:CG	1:B:951:LEU:HD12	2.50	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	896/970 (92%)	775 (86%)	103 (12%)	18 (2%)	9	39
1	B	896/970 (92%)	742 (83%)	123 (14%)	31 (4%)	4	23
All	All	1792/1940 (92%)	1517 (85%)	226 (13%)	49 (3%)	6	30

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	ASP
1	A	674	GLY
1	A	773	ARG
1	A	794	VAL
1	A	949	PRO
1	B	476	GLY
1	B	674	GLY

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Mol	Chain	Res	Type
1	B	949	PRO
1	A	155	GLY
1	A	272	ILE
1	A	450	LEU
1	A	554	GLY
1	A	556	ARG
1	A	943	PRO
1	B	269	ASN
1	B	289	MET
1	B	330	LEU
1	B	739	VAL
1	B	846	GLU
1	A	496	GLY
1	B	450	LEU
1	B	499	PRO
1	B	556	ARG
1	B	679	PHE
1	B	728	TYR
1	B	753	ARG
1	B	852	GLU
1	B	943	PRO
1	B	948	PRO
1	A	120	ARG
1	A	206	THR
1	B	122	ARG
1	B	270	ILE
1	B	298	ARG
1	B	350	SER
1	B	554	GLY
1	B	665	ASN
1	B	794	VAL
1	A	684	GLU
1	B	792	LEU
1	B	181	SER
1	A	178	PRO
1	B	272	ILE
1	A	354	VAL
1	B	475	ILE
1	B	666	GLY
1	A	475	ILE
1	B	921	PRO
1	B	756	ILE

### 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	781/831 (94%)	712 (91%)	69 (9%)	12	41
1	B	781/831 (94%)	718 (92%)	63 (8%)	14	45
All	All	1562/1662 (94%)	1430 (92%)	132 (8%)	12	43

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	TYR
1	A	41	LEU
1	A	58	ARG
1	A	78	THR
1	A	141	SER
1	A	145	GLU
1	A	183	ARG
1	A	188	GLN
1	A	207	ASP
1	A	209	ASP
1	A	213	LEU
1	A	226	ARG
1	A	232	ARG
1	A	238	GLN
1	A	241	MET
1	A	251	THR
1	A	260	LEU
1	A	273	ASN
1	A	283	ILE
1	A	302	GLU
1	A	322	GLN
1	A	328	PHE
1	A	332	MET
1	A	336	ASN
1	A	354	VAL
1	A	355	THR
1	A	387	GLU

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Mol	Chain	Res	Type
1	A	388	ARG
1	A	403	GLU
1	A	404	SER
1	A	407	THR
1	A	426	CYS
1	A	456	ARG
1	A	497	LYS
1	A	513	ASP
1	A	514	VAL
1	A	556	ARG
1	A	559	LEU
1	A	567	ARG
1	A	585	ASP
1	A	590	ARG
1	A	603	ASP
1	A	604	SER
1	A	606	LYS
1	A	612	SER
1	A	624	MET
1	A	633	VAL
1	A	636	THR
1	A	662	ASP
1	A	678	GLU
1	A	687	CYS
1	A	689	GLN
1	A	712	GLU
1	A	714	ARG
1	A	717	MET
1	A	735	GLU
1	A	799	LYS
1	A	810	GLN
1	A	845	ASP
1	A	853	LEU
1	A	861	ARG
1	A	869	GLN
1	A	893	LEU
1	A	904	PHE
1	A	938	LEU
1	A	941	LEU
1	A	949	PRO
1	A	957	LEU
1	A	967	GLN

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Mol	Chain	Res	Type
1	B	37	TYR
1	B	74	LYS
1	B	82	GLU
1	B	116	GLN
1	B	188	GLN
1	B	197	LEU
1	B	207	ASP
1	B	232	ARG
1	B	238	GLN
1	B	254	LYS
1	B	260	LEU
1	B	270	ILE
1	B	273	ASN
1	B	281	SER
1	B	283	ILE
1	B	288	TRP
1	B	302	GLU
1	B	306	ASP
1	B	324	GLU
1	B	328	PHE
1	B	332	MET
1	B	336	ASN
1	B	381	LYS
1	B	385	THR
1	B	387	GLU
1	B	388	ARG
1	B	437	LEU
1	B	456	ARG
1	B	458	GLU
1	B	469	ILE
1	B	497	LYS
1	B	556	ARG
1	B	564	LEU
1	B	568	LEU
1	B	585	ASP
1	B	589	ASP
1	B	590	ARG
1	B	597	VAL
1	B	606	LYS
1	B	624	MET
1	B	636	THR
1	B	638	PHE

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Mol	Chain	Res	Type
1	B	645	VAL
1	B	662	ASP
1	B	678	GLU
1	B	687	CYS
1	B	707	VAL
1	B	714	ARG
1	B	726	GLU
1	B	742	PHE
1	B	770	THR
1	B	773	ARG
1	B	777	TRP
1	B	783	GLN
1	B	806	VAL
1	B	852	GLU
1	B	853	LEU
1	B	854	LYS
1	B	869	GLN
1	B	904	PHE
1	B	928	GLU
1	B	949	PRO
1	B	953	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	116	GLN
1	A	167	ASN
1	A	188	GLN
1	A	190	ASN
1	A	195	ASN
1	A	199	GLN
1	A	201	ASN
1	A	238	GLN
1	A	273	ASN
1	A	336	ASN
1	A	384	ASN
1	A	507	GLN
1	A	595	GLN
1	A	626	GLN
1	A	653	HIS
1	A	692	GLN

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Mol	Chain	Res	Type
1	A	701	HIS
1	A	755	ASN
1	A	783	GLN
1	A	873	GLN
1	A	895	ASN
1	A	905	GLN
1	A	922	GLN
1	A	967	GLN
1	B	47	ASN
1	B	110	ASN
1	B	116	GLN
1	B	180	GLN
1	B	188	GLN
1	B	190	ASN
1	B	238	GLN
1	B	249	HIS
1	B	273	ASN
1	B	317	ASN
1	B	336	ASN
1	B	368	ASN
1	B	572	GLN
1	B	626	GLN
1	B	653	HIS
1	B	673	GLN
1	B	689	GLN
1	B	701	HIS
1	B	755	ASN
1	B	783	GLN
1	B	868	GLN
1	B	895	ASN
1	B	905	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	971	-	4,4,4	0.30	0	6,6,6	0.17	0
2	SO4	B	1071	-	4,4,4	0.29	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	971	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1071	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	971	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	904/970 (93%)	-0.51	0 100 100	16, 49, 88, 122	0
1	B	904/970 (93%)	-0.47	0 100 100	23, 63, 102, 132	0
All	All	1808/1940 (93%)	-0.49	0 100 100	16, 56, 98, 132	0

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	971	5/5	0.98	0.16	-	50,50,51,52	0
2	SO4	B	1071	5/5	0.98	0.10	-	88,88,89,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.