Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 06:36 AM EST

PDB ID	:	1T70
Title	:	Crystal structure of a novel phosphatase from Deinococcus radiodurans
Authors	:	Shin, D.H.; Wang, W.; Kim, R.; Yokota, H.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2004-05-07
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

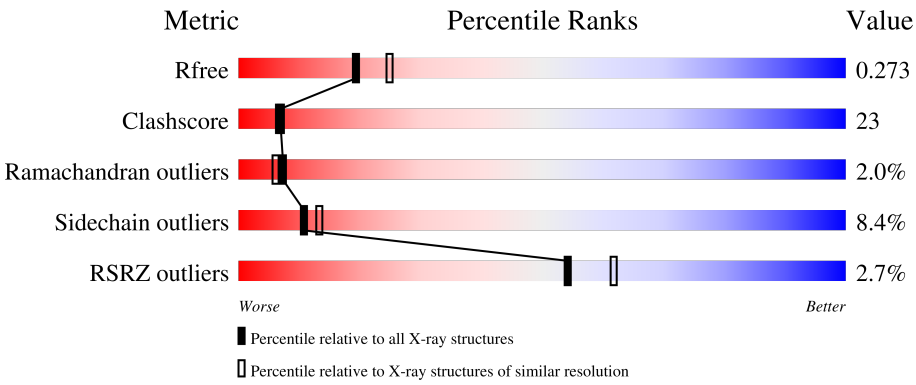
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	255	64% 31% 5%
1	B	255	% 63% 33% •
1	C	255	2% 63% 32% 5%
1	D	255	4% 63% 31% 5%
1	E	255	3% 59% 35% 6%

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Mol	Chain	Length	Quality of chain
1	F	255	3% 59% 36%
1	G	255	7% 50% 44% 6%
1	H	255	2% 62% 33% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16095 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 Phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	1972	1243	358	363	8	0	0	0
1	B	255	1972	1243	358	363	8	0	0	0
1	C	255	1972	1243	358	363	8	0	0	0
1	D	255	1972	1243	358	363	8	0	0	0
1	E	255	1972	1243	358	363	8	0	0	0
1	F	255	1972	1243	358	363	8	0	0	0
1	G	255	1972	1243	358	363	8	0	0	0
1	H	255	1972	1243	358	363	8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	58	58	58	0	0
2	B	56	56	56	0	0
2	C	55	55	55	0	0
2	D	39	39	39	0	0
2	E	26	26	26	0	0
2	F	42	42	42	0	0

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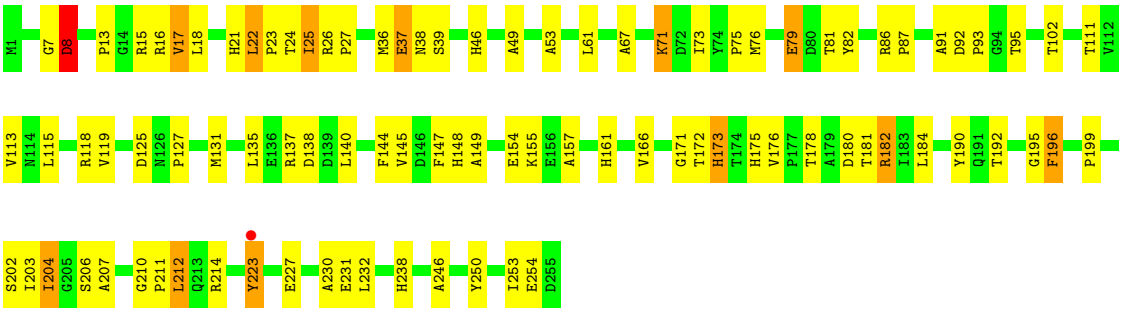
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	G	16	16	16	0	0
			Total	O		
2	H	27	27	27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

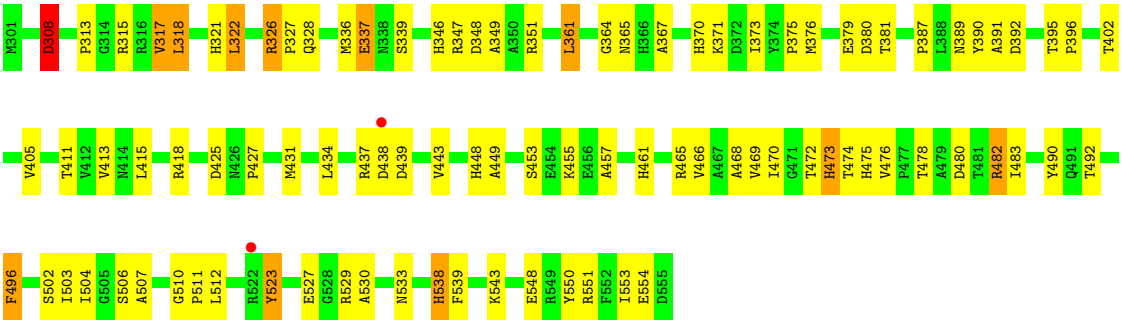
• Molecule 1: Phosphatase

Chain A: 64% 31% 5%



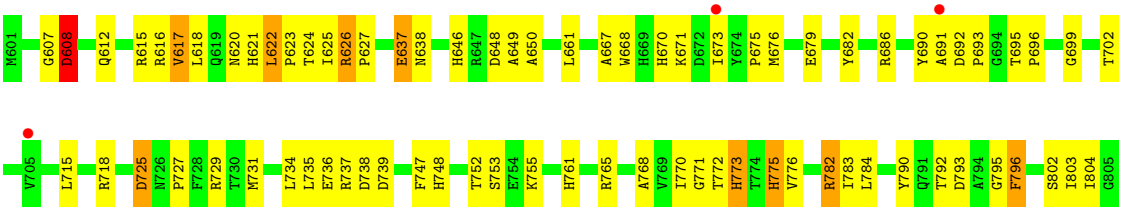
• Molecule 1: Phosphatase

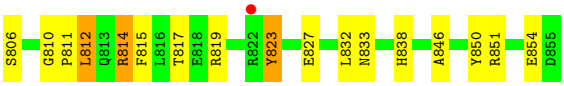
Chain B: % 63% 33% •



• Molecule 1: Phosphatase

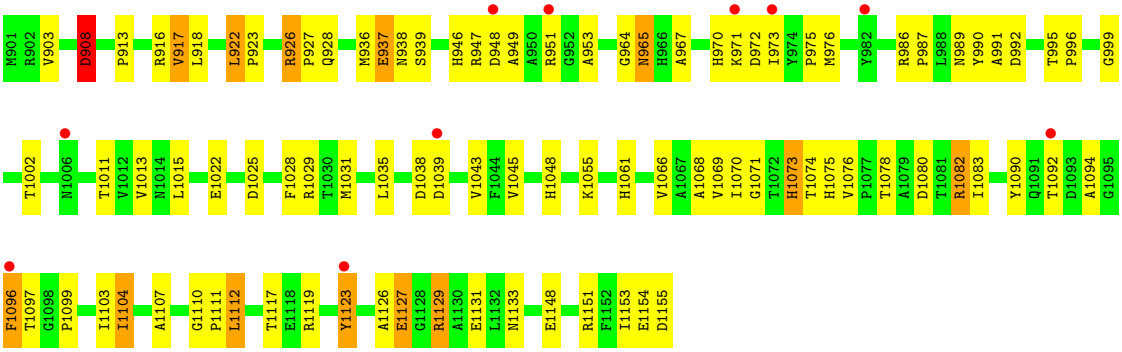
Chain C: 2% 63% 32% 5%





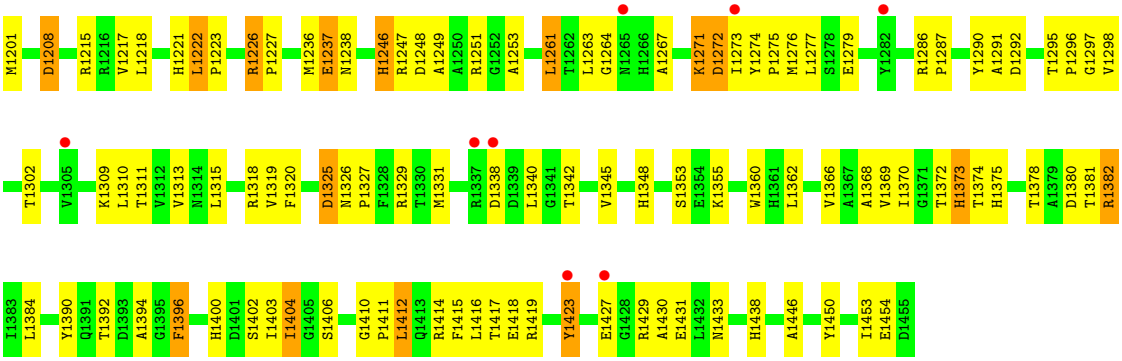
- Molecule 1: Phosphatase

Chain D:



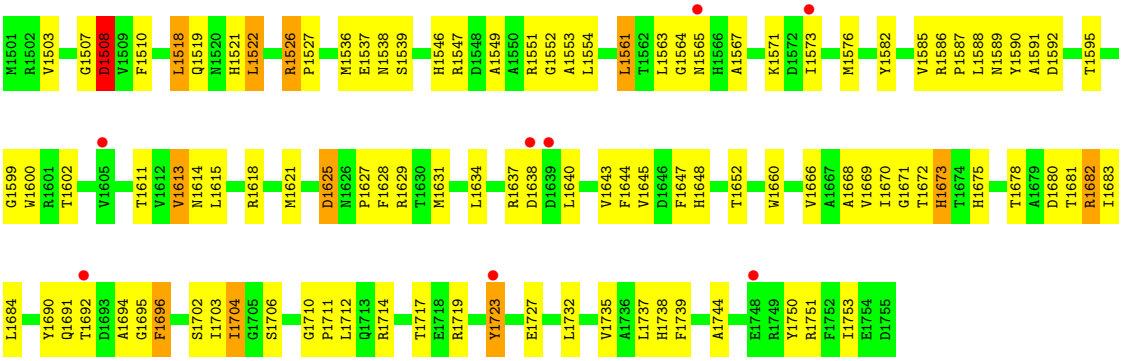
- Molecule 1: Phosphatase

Chain E:



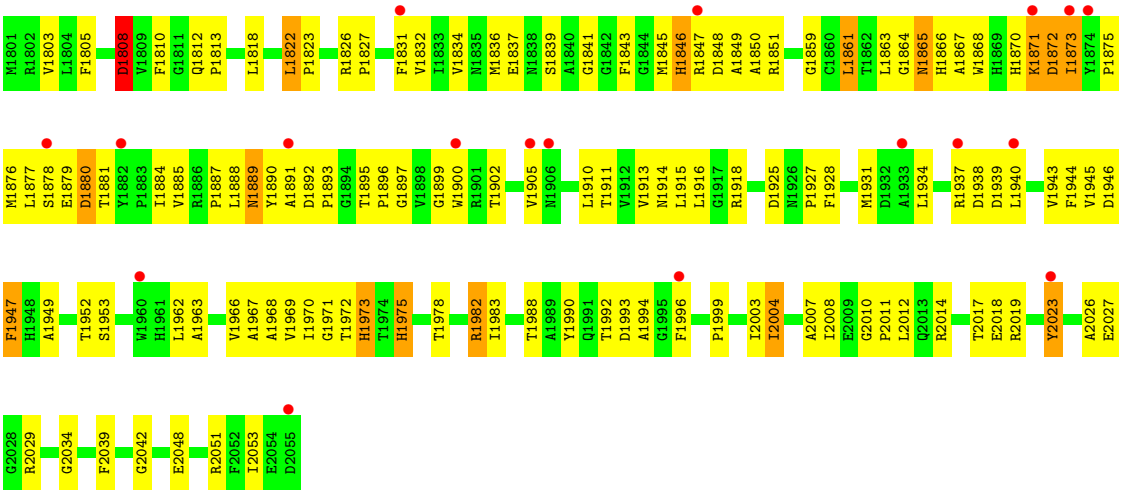
- Molecule 1: Phosphatase

Chain F:



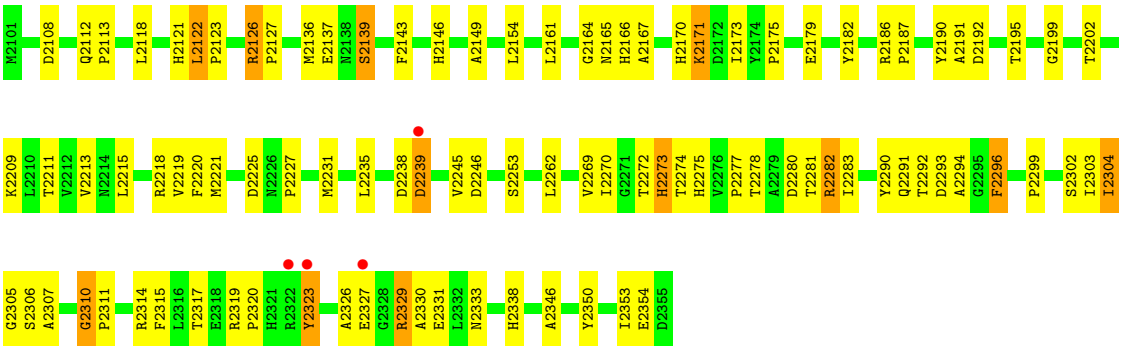
- Molecule 1: Phosphatase

Chain G:



- Molecule 1: Phosphatase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	242.79Å 116.61Å 89.28Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	19.95 – 2.30 47.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.5 (19.95-2.30) 90.2 (47.54-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.260 0.222 , 0.273	Depositor DCC
R_{free} test set	10028 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16095	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	0/2022	0.66	0/2743
1	B	0.39	0/2022	0.67	0/2743
1	C	0.36	0/2022	0.67	0/2743
1	D	0.37	0/2022	0.65	0/2743
1	E	0.35	0/2022	0.62	0/2743
1	F	0.37	0/2022	0.65	0/2743
1	G	0.35	0/2022	0.62	0/2743
1	H	0.37	0/2022	0.63	0/2743
All	All	0.37	0/16176	0.65	0/21944

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 (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	1972	0	1904	76	0
1	B	1972	0	1901	85	0
1	C	1972	0	1901	102	0
1	D	1972	0	1901	107	0
1	E	1972	0	1901	108	0
1	F	1972	0	1901	96	0
1	G	1972	0	1901	129	0
1	H	1972	0	1901	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	58	0	0	1	0
2	B	56	0	0	2	0
2	C	55	0	0	2	0
2	D	39	0	0	5	0
2	E	26	0	0	2	0
2	F	42	0	0	1	0
2	G	16	0	0	0	0
2	H	27	0	0	0	0
All	All	16095	0	15211	713	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (713) 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:C:729:ARG:NH2	1:E:1291:ALA:HB3	1.67	1.09
1:D:991:ALA:HB3	1:F:1629:ARG:HH22	1.08	1.08
1:C:729:ARG:HH22	1:E:1291:ALA:HB3	0.97	1.08
1:D:1029:ARG:HH22	1:F:1591:ALA:HB3	0.98	1.07
1:C:667:ALA:O	1:C:673:ILE:HD13	1.63	0.98
1:D:992:ASP:HB3	1:D:995:THR:HG23	1.47	0.97
1:A:67:ALA:O	1:A:73:ILE:HD13	1.64	0.96
1:D:1029:ARG:NH2	1:F:1591:ALA:HB3	1.80	0.95
1:A:25:ILE:HG23	1:D:1148:GLU:OE1	1.66	0.94
1:B:548:GLU:OE1	1:C:625:ILE:HG23	1.66	0.94
1:D:991:ALA:HB3	1:F:1629:ARG:NH2	1.83	0.94
1:F:1567:ALA:O	1:F:1573:ILE:HD13	1.68	0.93
1:D:967:ALA:O	1:D:973:ILE:HD13	1.67	0.93
1:E:1382:ARG:HH11	1:E:1382:ARG:HB3	1.32	0.91
1:E:1267:ALA:O	1:E:1273:ILE:HD13	1.72	0.89
1:H:2170:HIS:O	1:H:2173:ILE:HD12	1.76	0.86
1:G:1945:VAL:HG21	1:G:1962:LEU:HD23	1.58	0.84
1:B:367:ALA:O	1:B:373:ILE:HD13	1.78	0.83
1:B:418:ARG:HD2	1:B:427:PRO:HD3	1.59	0.82
1:D:1080:ASP:OD1	1:D:1092:THR:HG23	1.80	0.82
1:G:1847:ARG:HA	1:G:1876:MET:HE1	1.61	0.82
1:E:1380:ASP:OD1	1:E:1392:THR:HG23	1.80	0.82
1:E:1315:LEU:HG	1:E:1331:MET:HE2	1.61	0.81
1:F:1547:ARG:HA	1:F:1576:MET:HE1	1.61	0.81
1:F:1602:THR:HG22	1:F:1611:THR:OG1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1868:TRP:HA	1:G:1873:ILE:HD13	1.62	0.81
1:H:2192:ASP:HB3	1:H:2195:THR:HG23	1.63	0.81
1:A:92:ASP:HB3	1:A:95:THR:HG23	1.64	0.80
1:B:548:GLU:HG2	1:C:624:THR:HB	1.64	0.80
1:C:621:HIS:HE1	1:C:850:TYR:OH	1.63	0.80
1:C:691:ALA:HB2	1:C:725:ASP:OD1	1.82	0.79
1:F:1591:ALA:HB2	1:F:1625:ASP:OD1	1.82	0.79
1:E:1247:ARG:HA	1:E:1276:MET:HE1	1.64	0.79
1:D:964:GLY:HA2	1:D:987:PRO:CG	2.14	0.78
1:B:490:TYR:OH	1:B:492:THR:HG22	1.81	0.78
1:E:1326:ASN:HB2	1:E:1329:ARG:HH21	1.49	0.77
1:A:46:HIS:HD2	1:A:49:ALA:H	1.29	0.77
1:B:391:ALA:HB2	1:B:425:ASP:CG	2.05	0.77
1:C:718:ARG:HD2	1:C:727:PRO:HD3	1.66	0.77
1:G:2051:ARG:HE	1:G:2053:ILE:HD11	1.49	0.76
1:E:1315:LEU:HD11	1:E:1331:MET:HG2	1.65	0.76
1:E:1375:HIS:HD2	1:E:1404:ILE:O	1.69	0.76
1:E:1292:ASP:HB3	1:E:1295:THR:HG23	1.68	0.76
1:F:1592:ASP:HB3	1:F:1595:THR:HG23	1.67	0.76
1:H:2213:VAL:HG21	1:H:2231:MET:HE1	1.68	0.76
1:D:991:ALA:CB	1:F:1629:ARG:HH22	1.95	0.75
1:C:729:ARG:HH22	1:E:1291:ALA:CB	1.90	0.75
1:H:2121:HIS:HE1	1:H:2350:TYR:OH	1.68	0.75
1:F:1690:TYR:OH	1:F:1692:THR:HG22	1.86	0.75
1:A:91:ALA:HB2	1:A:125:ASP:CG	2.07	0.75
1:H:2167:ALA:O	1:H:2173:ILE:HD13	1.86	0.75
1:E:1382:ARG:HH11	1:E:1382:ARG:CB	1.99	0.75
1:C:692:ASP:N	1:E:1329:ARG:NH1	2.36	0.74
1:B:434:LEU:HD12	1:B:437:ARG:HE	1.53	0.74
1:A:190:TYR:OH	1:A:192:THR:HG22	1.89	0.73
1:E:1302:THR:HG22	1:E:1311:THR:OG1	1.88	0.73
1:G:1822:LEU:HD11	1:G:1832:VAL:HG11	1.71	0.73
1:G:1867:ALA:O	1:G:1873:ILE:HD13	1.88	0.73
1:D:964:GLY:HA2	1:D:987:PRO:HG3	1.71	0.72
1:A:46:HIS:CD2	1:A:49:ALA:H	2.07	0.72
1:H:2282:ARG:HH11	1:H:2282:ARG:HB3	1.53	0.72
1:C:646:HIS:CD2	1:C:649:ALA:H	2.08	0.72
1:E:1390:TYR:OH	1:E:1392:THR:HG22	1.90	0.72
1:B:347:ARG:HA	1:B:376:MET:HE1	1.71	0.72
1:D:1090:TYR:OH	1:D:1092:THR:HG22	1.90	0.72
1:B:415:LEU:HG	1:B:431:MET:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1846:HIS:HD2	1:G:1849:ALA:H	1.37	0.72
1:G:1861:LEU:N	1:G:1861:LEU:HD22	2.05	0.72
1:B:375:PRO:O	1:B:379:GLU:HG2	1.90	0.71
1:C:782:ARG:HH11	1:C:782:ARG:HB3	1.54	0.71
1:E:1416:LEU:HD23	1:F:1629:ARG:HG3	1.72	0.71
1:C:646:HIS:HD2	1:C:649:ALA:H	1.38	0.70
1:G:1889:ASN:HB2	1:G:1925:ASP:O	1.91	0.70
1:G:1846:HIS:CD2	1:G:1849:ALA:H	2.09	0.70
1:A:24:THR:HB	1:D:1148:GLU:HG2	1.71	0.70
1:C:692:ASP:HB3	1:C:695:THR:HG23	1.74	0.70
1:G:1803:VAL:HG21	1:G:2039:PHE:CE2	2.27	0.70
1:C:691:ALA:HB3	1:E:1329:ARG:NH1	2.06	0.69
1:C:718:ARG:HD2	1:C:727:PRO:CD	2.22	0.69
1:H:2191:ALA:HB2	1:H:2225:ASP:OD1	1.91	0.69
1:A:161:HIS:HB2	1:B:512:LEU:HD21	1.73	0.69
1:C:675:PRO:O	1:C:679:GLU:HG2	1.93	0.68
1:B:379:GLU:O	1:B:381:THR:HG23	1.92	0.68
1:G:1836:MET:HB3	1:G:1839:SER:OG	1.94	0.68
1:G:2011:PRO:HG3	1:G:2023:TYR:HD1	1.59	0.68
1:A:178:THR:HG21	1:A:192:THR:OG1	1.93	0.68
1:F:1680:ASP:OD1	1:F:1692:THR:HG23	1.93	0.68
1:G:1864:GLY:HA2	1:G:1887:PRO:HG3	1.75	0.68
1:B:503:ILE:O	1:B:504:ILE:HG22	1.93	0.68
1:G:1847:ARG:HA	1:G:1876:MET:CE	2.23	0.67
1:C:691:ALA:HB3	1:E:1329:ARG:HH12	1.58	0.67
1:D:1015:LEU:HD11	1:D:1031:MET:HG2	1.75	0.67
1:E:1438:HIS:HB2	1:E:1446:ALA:HB3	1.77	0.67
1:F:1546:HIS:HD2	1:F:1549:ALA:H	1.41	0.67
1:D:1029:ARG:HH12	1:F:1591:ALA:HB1	1.60	0.67
1:E:1403:ILE:O	1:E:1404:ILE:HG22	1.94	0.67
1:H:2290:TYR:OH	1:H:2292:THR:HG22	1.95	0.67
1:A:8:ASP:HB3	1:A:38:ASN:HD22	1.58	0.66
1:A:25:ILE:HG23	1:D:1148:GLU:CD	2.14	0.66
1:A:75:PRO:O	1:A:79:GLU:HG2	1.94	0.66
1:A:202:SER:HB2	1:A:206:SER:O	1.94	0.66
1:F:1546:HIS:CD2	1:F:1549:ALA:H	2.13	0.66
1:H:2280:ASP:OD1	1:H:2292:THR:HG23	1.94	0.66
1:A:21:HIS:HE1	1:A:250:TYR:OH	1.79	0.66
1:A:204:ILE:HD12	1:B:453:SER:HB3	1.77	0.66
1:G:1990:TYR:OH	1:G:1992:THR:HG22	1.95	0.66
1:D:1103:ILE:O	1:D:1104:ILE:HG22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1871:LYS:HG2	1:G:1872:ASP:N	2.10	0.66
1:A:79:GLU:O	1:A:81:THR:HG23	1.96	0.65
1:G:2004:ILE:HD12	1:H:2253:SER:HB3	1.77	0.65
1:H:2215:LEU:HD11	1:H:2231:MET:HG2	1.77	0.65
1:D:991:ALA:HB1	1:F:1629:ARG:HH12	1.60	0.65
1:F:1618:ARG:HD2	1:F:1627:PRO:HD3	1.79	0.65
1:D:1015:LEU:HD11	1:D:1031:MET:CG	2.26	0.65
1:B:418:ARG:HD2	1:B:427:PRO:CD	2.26	0.65
1:G:1879:GLU:O	1:G:1881:THR:HG23	1.96	0.65
1:H:2275:HIS:HD2	1:H:2304:ILE:O	1.79	0.65
1:D:936:MET:HB3	1:D:939:SER:OG	1.98	0.64
1:E:1222:LEU:N	1:E:1223:PRO:HD2	2.10	0.64
1:G:1967:ALA:HB1	1:G:2039:PHE:CE1	2.32	0.64
1:G:1902:THR:HG22	1:G:1911:THR:OG1	1.98	0.64
1:F:1703:ILE:O	1:F:1704:ILE:HG22	1.97	0.64
1:E:1291:ALA:HB2	1:E:1325:ASP:OD1	1.97	0.64
1:D:1066:VAL:HG12	1:D:1068:ALA:H	1.63	0.64
1:E:1237:GLU:HG2	1:E:1238:ASN:ND2	2.13	0.64
1:F:1710:GLY:HA3	1:F:1723:TYR:HB3	1.80	0.64
1:E:1378:THR:HG21	1:E:1392:THR:OG1	1.97	0.63
1:E:1315:LEU:HG	1:E:1331:MET:CE	2.29	0.63
1:E:1326:ASN:CB	1:E:1329:ARG:HH21	2.10	0.63
1:H:2202:THR:HG22	1:H:2211:THR:OG1	1.99	0.63
1:A:176:VAL:HG21	1:B:492:THR:HG21	1.81	0.63
1:A:210:GLY:HA3	1:A:223:TYR:HB3	1.80	0.63
1:B:482:ARG:HB3	1:B:482:ARG:HH11	1.64	0.63
1:F:1643:VAL:O	1:F:1666:VAL:HG13	1.99	0.63
1:F:1735:VAL:HG12	1:F:1737:LEU:HD21	1.81	0.62
1:E:1247:ARG:HA	1:E:1276:MET:CE	2.30	0.62
1:E:1372:THR:O	1:E:1373:HIS:HB3	1.99	0.62
1:G:1843:PHE:HD1	1:G:1866:HIS:CD2	2.17	0.62
1:H:2215:LEU:HG	1:H:2231:MET:CE	2.30	0.62
1:F:1675:HIS:HD2	1:F:1704:ILE:O	1.83	0.62
1:G:1913:VAL:HG11	1:G:1931:MET:HE1	1.79	0.62
1:G:1872:ASP:O	1:G:1876:MET:HG3	1.99	0.62
1:G:1953:SER:HB3	1:H:2304:ILE:HD12	1.81	0.62
1:H:2191:ALA:HB2	1:H:2225:ASP:CG	2.20	0.62
1:B:321:HIS:HE1	1:B:550:TYR:OH	1.82	0.62
1:B:351:ARG:HD2	2:B:583:HOH:O	1.99	0.62
1:G:1947:PHE:O	1:G:1971:GLY:HA2	2.00	0.62
1:H:2215:LEU:HG	1:H:2231:MET:HE2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2338:HIS:HB2	1:H:2346:ALA:HB3	1.80	0.62
1:A:172:THR:O	1:A:173:HIS:HB3	1.98	0.62
1:D:1029:ARG:HH12	1:F:1591:ALA:CB	2.12	0.62
1:D:1110:GLY:HA3	1:D:1123:TYR:HB3	1.81	0.61
1:E:1275:PRO:O	1:E:1279:GLU:HG2	2.00	0.61
1:G:1864:GLY:HA2	1:G:1887:PRO:CG	2.30	0.61
1:C:612:GLN:HG3	1:C:615:ARG:NH2	2.15	0.61
1:G:1803:VAL:HG21	1:G:2039:PHE:HE2	1.65	0.61
1:D:946:HIS:HD2	1:D:949:ALA:H	1.49	0.61
1:A:180:ASP:OD1	1:A:192:THR:HG23	2.00	0.61
1:H:2121:HIS:CE1	1:H:2350:TYR:OH	2.54	0.60
1:B:478:THR:HG21	1:B:492:THR:OG1	2.01	0.60
1:E:1414:ARG:HD2	2:E:185:HOH:O	2.01	0.60
1:A:212:LEU:HD21	1:B:461:HIS:HB2	1.84	0.60
1:B:391:ALA:HB2	1:B:425:ASP:OD1	2.00	0.60
1:G:1891:ALA:HB2	1:G:1925:ASP:OD1	2.02	0.60
1:G:1975:HIS:O	1:G:1996:PHE:HB2	2.01	0.60
1:E:1246:HIS:CD2	1:E:1249:ALA:H	2.20	0.59
1:E:1366:VAL:HG12	1:E:1368:ALA:H	1.67	0.59
1:H:2215:LEU:HD11	1:H:2231:MET:CG	2.32	0.59
1:B:480:ASP:OD1	1:B:492:THR:HG23	2.02	0.59
1:C:621:HIS:CE1	1:C:850:TYR:OH	2.52	0.59
1:B:415:LEU:HD11	1:B:431:MET:HG2	1.84	0.59
1:H:2219:VAL:HG12	1:H:2220:PHE:CD2	2.36	0.59
1:C:692:ASP:N	1:E:1329:ARG:HH12	1.99	0.59
1:H:2282:ARG:HH11	1:H:2282:ARG:CB	2.16	0.59
1:B:523:TYR:N	1:B:523:TYR:CD2	2.69	0.59
1:E:1311:THR:HG21	1:E:1340:LEU:HD22	1.85	0.59
1:H:2319:ARG:HB3	1:H:2320:PRO:HD2	1.85	0.59
1:D:1078:THR:HG21	1:D:1092:THR:OG1	2.02	0.59
1:E:1375:HIS:CD2	1:E:1404:ILE:HG12	2.38	0.59
1:A:27:PRO:HA	1:D:928:GLN:HE22	1.67	0.58
1:H:2272:THR:O	1:H:2273:HIS:HB3	2.03	0.58
1:D:1075:HIS:O	1:D:1096:PHE:HB2	2.03	0.58
1:F:1672:THR:O	1:F:1673:HIS:HB3	2.03	0.58
1:A:182:ARG:HH11	1:A:182:ARG:HB3	1.69	0.58
1:C:772:THR:O	1:C:773:HIS:HB3	2.03	0.58
1:G:1826:ARG:O	1:G:1826:ARG:HD3	2.03	0.58
1:C:715:LEU:HD11	1:C:731:MET:HG2	1.84	0.58
1:E:1353:SER:HB3	1:F:1704:ILE:HD12	1.84	0.58
1:G:1847:ARG:HG2	1:G:1851:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1682:ARG:HG2	1:F:1683:ILE:H	1.66	0.58
1:G:1945:VAL:HG21	1:G:1962:LEU:CD2	2.33	0.58
1:C:670:HIS:O	1:C:673:ILE:HD12	2.04	0.58
1:G:1971:GLY:O	1:G:1993:ASP:HA	2.02	0.58
1:D:916:ARG:NH1	1:D:1154:GLU:OE1	2.37	0.58
1:D:1099:PRO:CB	1:D:1126:ALA:HB3	2.33	0.58
1:E:1246:HIS:HD2	1:E:1249:ALA:H	1.49	0.58
1:G:1839:SER:HB2	1:G:1845:MET:HA	1.86	0.58
1:A:25:ILE:HA	1:D:1148:GLU:OE2	2.03	0.57
1:D:972:ASP:O	1:D:976:MET:HG3	2.04	0.57
1:D:913:PRO:O	1:D:917:VAL:HG22	2.03	0.57
1:G:1848:ASP:HA	1:G:1851:ARG:NH1	2.19	0.57
1:C:782:ARG:HG2	1:C:783:ILE:H	1.68	0.57
1:H:2190:TYR:HB3	1:H:2195:THR:HG21	1.86	0.57
1:C:753:SER:HB3	1:D:1104:ILE:HD12	1.86	0.57
1:D:948:ASP:HA	1:D:951:ARG:HH12	1.70	0.57
1:A:91:ALA:HB2	1:A:125:ASP:OD1	2.05	0.57
1:E:1236:MET:HG3	1:E:1261:LEU:HG	1.86	0.57
1:H:2218:ARG:HD2	1:H:2227:PRO:HD2	1.87	0.57
1:H:2329:ARG:HD2	1:H:2354:GLU:O	2.05	0.57
1:C:718:ARG:HD3	2:C:163:HOH:O	2.04	0.57
1:A:115:LEU:HD11	1:A:131:MET:HG2	1.87	0.57
1:D:1075:HIS:HD2	1:D:1104:ILE:HG12	1.70	0.57
1:G:1949:ALA:O	1:G:1973:HIS:HB3	2.05	0.57
1:A:203:ILE:O	1:A:204:ILE:HG22	2.05	0.56
1:E:1375:HIS:CD2	1:E:1404:ILE:O	2.55	0.56
1:G:2011:PRO:HG3	1:G:2023:TYR:CD1	2.39	0.56
1:A:182:ARG:HH11	1:A:182:ARG:CB	2.19	0.56
1:D:1111:PRO:HG3	1:D:1123:TYR:CD1	2.40	0.56
1:F:1588:LEU:HD22	1:F:1634:LEU:HD22	1.86	0.56
1:G:2003:ILE:O	1:G:2004:ILE:HG22	2.05	0.56
1:C:833:ASN:OD1	1:C:851:ARG:HG3	2.06	0.56
1:F:1675:HIS:O	1:F:1696:PHE:HB2	2.04	0.56
1:B:548:GLU:OE2	1:C:625:ILE:HA	2.04	0.56
1:F:1670:ILE:N	1:F:1670:ILE:HD12	2.21	0.56
1:D:948:ASP:HA	1:D:951:ARG:NH1	2.21	0.56
1:F:1589:ASN:O	1:F:1625:ASP:HB2	2.04	0.56
1:H:2310:GLY:HA3	1:H:2323:TYR:HB3	1.87	0.56
1:D:1082:ARG:HH11	1:D:1082:ARG:HB3	1.70	0.56
1:H:2303:ILE:O	1:H:2304:ILE:HG22	2.06	0.56
1:B:402:THR:HG22	1:B:411:THR:OG1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:THR:O	1:B:473:HIS:HB3	2.06	0.56
1:D:1013:VAL:CG1	1:D:1045:VAL:HG22	2.36	0.56
1:E:1272:ASP:O	1:E:1275:PRO:HG2	2.06	0.56
1:G:1915:LEU:HD11	1:G:1931:MET:HG2	1.88	0.56
1:G:1803:VAL:HG12	1:G:1831:PHE:HB3	1.87	0.55
1:D:1082:ARG:HG2	2:D:52:HOH:O	2.06	0.55
1:G:1982:ARG:HG2	1:G:1983:ILE:H	1.70	0.55
1:B:326:ARG:O	1:B:326:ARG:HD3	2.06	0.55
1:G:1812:GLN:HB2	1:G:1813:PRO:HD3	1.87	0.55
1:H:2112:GLN:HB2	1:H:2113:PRO:HD3	1.89	0.55
1:A:118:ARG:HD2	1:A:127:PRO:CD	2.36	0.55
1:F:1615:LEU:HG	1:F:1631:MET:HE3	1.87	0.55
1:F:1735:VAL:CG1	1:F:1737:LEU:HD21	2.37	0.55
1:E:1217:VAL:HG12	1:E:1454:GLU:OE2	2.07	0.55
1:B:548:GLU:CD	1:C:625:ILE:HG23	2.26	0.55
1:D:946:HIS:CD2	1:D:949:ALA:H	2.24	0.55
1:D:1129:ARG:HD2	1:D:1155:ASP:OXT	2.06	0.55
1:E:1271:LYS:O	1:E:1275:PRO:HD2	2.05	0.55
1:E:1277:LEU:HD22	1:E:1297:GLY:HA3	1.88	0.55
1:H:2175:PRO:O	1:H:2179:GLU:HG2	2.06	0.55
1:E:1423:TYR:HD2	1:E:1423:TYR:O	1.89	0.55
1:D:1043:VAL:O	1:D:1066:VAL:HG13	2.06	0.54
1:F:1735:VAL:HG12	1:F:1737:LEU:CD2	2.37	0.54
1:G:1826:ARG:HG2	1:G:1832:VAL:HG21	1.88	0.54
1:D:1015:LEU:HD21	1:D:1031:MET:HE2	1.89	0.54
1:F:1669:VAL:C	1:F:1670:ILE:HD12	2.28	0.54
1:G:1999:PRO:HG3	1:G:2026:ALA:HB3	1.88	0.54
1:E:1431:GLU:HB2	1:E:1453:ILE:HD13	1.89	0.54
1:F:1536:MET:HE2	1:F:1553:ALA:HB2	1.89	0.54
1:H:2146:HIS:CD2	1:H:2149:ALA:H	2.26	0.54
1:A:113:VAL:HG12	1:A:144:PHE:O	2.08	0.54
1:B:482:ARG:HH11	1:B:482:ARG:CB	2.20	0.54
1:G:1970:ILE:N	1:G:1970:ILE:HD12	2.22	0.54
1:G:2023:TYR:CD2	1:G:2023:TYR:N	2.74	0.54
1:G:1888:LEU:CD1	1:G:1899:GLY:HA3	2.38	0.53
1:A:91:ALA:HB2	1:A:125:ASP:OD2	2.08	0.53
1:C:752:THR:HG21	1:D:1074:THR:HB	1.89	0.53
1:D:1002:THR:HG22	1:D:1011:THR:OG1	2.09	0.53
1:C:729:ARG:NH2	1:E:1291:ALA:CB	2.57	0.53
1:G:2007:ALA:O	1:G:2011:PRO:HD2	2.09	0.53
1:B:469:VAL:C	1:B:470:ILE:HD12	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:HIS:HB2	1:C:846:ALA:HB3	1.90	0.53
1:A:7:GLY:HA3	1:A:195:GLY:O	2.08	0.53
1:C:782:ARG:HG2	1:C:783:ILE:N	2.23	0.53
1:D:1013:VAL:HG21	1:D:1031:MET:CE	2.39	0.53
1:A:137:ARG:HD2	1:A:140:LEU:HD21	1.90	0.53
1:B:548:GLU:CG	1:C:624:THR:HB	2.35	0.53
1:C:782:ARG:HH11	1:C:782:ARG:CB	2.22	0.53
1:D:1013:VAL:HG21	1:D:1031:MET:HE1	1.91	0.53
1:H:2113:PRO:HB2	1:H:2299:PRO:HD3	1.90	0.53
1:G:1943:VAL:O	1:G:1966:VAL:HG13	2.09	0.52
1:G:1945:VAL:HG23	1:G:1966:VAL:HG11	1.90	0.52
1:A:172:THR:O	1:A:173:HIS:CB	2.58	0.52
1:E:1287:PRO:HB2	1:E:1290:TYR:CE2	2.43	0.52
1:C:810:GLY:HA3	1:C:823:TYR:HB3	1.92	0.52
1:D:1148:GLU:HB3	2:D:69:HOH:O	2.08	0.52
1:G:1818:LEU:HD13	1:G:1818:LEU:O	2.09	0.52
1:G:1978:THR:HA	1:H:2278:THR:HA	1.91	0.52
1:E:1374:THR:HB	1:F:1652:THR:HG21	1.91	0.52
1:F:1618:ARG:HD2	1:F:1627:PRO:CD	2.40	0.52
1:G:2023:TYR:H	1:G:2023:TYR:HD2	1.54	0.52
1:A:16:ARG:NH1	1:A:254:GLU:OE1	2.41	0.52
1:E:1402:SER:HB2	1:E:1406:SER:O	2.10	0.52
1:G:1891:ALA:HB2	1:G:1925:ASP:HB2	1.91	0.52
1:C:802:SER:HB2	1:C:806:SER:O	2.10	0.52
1:E:1372:THR:O	1:E:1373:HIS:CB	2.57	0.52
1:B:523:TYR:H	1:B:523:TYR:HD2	1.57	0.52
1:C:616:ARG:NH1	1:C:854:GLU:OE1	2.42	0.52
1:C:691:ALA:CB	1:E:1329:ARG:HH12	2.23	0.52
1:E:1355:LYS:HD3	1:E:1392:THR:O	2.10	0.52
1:F:1678:THR:HG21	1:F:1692:THR:OG1	2.09	0.52
1:B:472:THR:O	1:B:473:HIS:CB	2.57	0.52
1:B:523:TYR:N	1:B:523:TYR:HD2	2.07	0.52
1:D:990:TYR:HB3	1:D:995:THR:HG21	1.91	0.52
1:D:995:THR:HG22	1:E:1419:ARG:HH11	1.74	0.52
1:G:1845:MET:HE2	1:G:1863:LEU:HD21	1.91	0.52
1:B:315:ARG:HD2	2:B:606:HOH:O	2.08	0.52
1:E:1411:PRO:HG3	1:E:1423:TYR:CD1	2.45	0.52
1:H:2302:SER:HB2	1:H:2306:SER:O	2.09	0.52
1:H:2330:ALA:O	1:H:2354:GLU:HG2	2.10	0.51
1:G:1969:VAL:C	1:G:1970:ILE:HD12	2.31	0.51
1:H:2272:THR:O	1:H:2273:HIS:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:ASP:OD1	1:C:772:THR:HB	2.11	0.51
1:A:8:ASP:HB3	1:A:38:ASN:ND2	2.24	0.51
1:B:392:ASP:O	1:B:395:THR:HG23	2.11	0.51
1:C:737:ARG:HG2	1:C:737:ARG:HH11	1.76	0.51
1:A:13:PRO:O	1:A:17:VAL:HG22	2.11	0.51
1:D:1131:GLU:OE2	1:D:1133:ASN:ND2	2.43	0.51
1:C:607:GLY:HA3	1:C:795:GLY:O	2.10	0.51
1:A:118:ARG:HD2	1:A:127:PRO:HD2	1.91	0.51
1:B:313:PRO:O	1:B:317:VAL:HG23	2.10	0.51
1:B:474:THR:O	1:B:475:HIS:HB2	2.10	0.51
1:F:1521:HIS:HE1	1:F:1750:TYR:OH	1.94	0.51
1:F:1563:LEU:C	1:F:1614:ASN:HD21	2.14	0.51
1:G:1818:LEU:HD13	1:G:1818:LEU:C	2.30	0.51
1:B:328:GLN:HE22	1:C:627:PRO:HA	1.75	0.51
1:F:1554:LEU:CD1	1:F:1582:TYR:HD2	2.24	0.51
1:C:686:ARG:O	1:C:699:GLY:HA2	2.12	0.50
1:A:238:HIS:HB2	1:A:246:ALA:HB3	1.92	0.50
1:E:1248:ASP:HA	1:E:1251:ARG:HH12	1.75	0.50
1:D:1055:LYS:HD3	1:D:1092:THR:O	2.10	0.50
1:F:1547:ARG:HG3	1:F:1576:MET:HE3	1.94	0.50
1:G:1972:THR:O	1:G:1973:HIS:CB	2.60	0.50
1:H:2202:THR:HA	1:H:2211:THR:HA	1.94	0.50
1:H:2215:LEU:CG	1:H:2231:MET:HE2	2.41	0.50
1:B:439:ASP:OD2	1:B:439:ASP:N	2.40	0.50
1:E:1221:HIS:HE1	1:E:1450:TYR:OH	1.95	0.50
1:G:1810:PHE:HB2	1:G:1996:PHE:CE2	2.46	0.50
1:G:1885:VAL:HG12	1:G:1914:ASN:HB2	1.93	0.50
1:G:2017:THR:HB	1:G:2019:ARG:NH1	2.26	0.50
1:H:2213:VAL:CG2	1:H:2231:MET:HE1	2.40	0.50
1:C:691:ALA:HB3	1:E:1329:ARG:CZ	2.41	0.50
1:B:548:GLU:OE2	1:C:624:THR:O	2.30	0.50
1:C:782:ARG:HD2	1:C:784:LEU:HD23	1.92	0.50
1:D:1071:GLY:HA3	1:D:1092:THR:O	2.11	0.50
1:F:1691:GLN:NE2	1:F:1694:ALA:HA	2.27	0.50
1:C:646:HIS:CD2	1:C:649:ALA:N	2.80	0.50
1:C:832:LEU:C	1:C:832:LEU:HD23	2.32	0.50
1:A:231:GLU:HB2	1:A:253:ILE:HD13	1.94	0.50
1:B:308:ASP:HB2	1:B:496:PHE:HB2	1.92	0.50
1:B:347:ARG:HA	1:B:376:MET:CE	2.42	0.50
1:G:1875:PRO:O	1:G:1879:GLU:HG2	2.11	0.50
1:G:1888:LEU:HD22	1:G:1934:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:H	1:A:254:GLU:HG2	1.77	0.50
1:C:650:ALA:CB	1:C:676:MET:HE1	2.42	0.50
1:G:1888:LEU:HD13	1:G:1899:GLY:HA3	1.93	0.50
1:H:2291:GLN:HE21	1:H:2294:ALA:HA	1.76	0.49
1:A:22:LEU:N	1:A:23:PRO:HD2	2.26	0.49
1:E:1431:GLU:OE2	1:E:1433:ASN:ND2	2.46	0.49
1:F:1526:ARG:O	1:F:1526:ARG:HD3	2.12	0.49
1:F:1634:LEU:HD12	1:F:1637:ARG:HE	1.76	0.49
1:F:1672:THR:O	1:F:1673:HIS:CB	2.59	0.49
1:G:1871:LYS:O	1:G:1875:PRO:HD2	2.12	0.49
1:A:21:HIS:CE1	1:A:250:TYR:OH	2.63	0.49
1:D:1075:HIS:CD2	1:D:1104:ILE:HG12	2.48	0.49
1:G:1928:PHE:CE2	1:H:2315:PHE:HB3	2.47	0.49
1:D:964:GLY:O	1:D:967:ALA:N	2.43	0.49
1:D:1048:HIS:CE1	1:D:1073:HIS:CD2	3.01	0.49
1:D:1111:PRO:HG3	1:D:1123:TYR:HD1	1.77	0.49
1:B:504:ILE:HG23	1:B:504:ILE:O	2.12	0.49
1:D:937:GLU:HG3	1:D:938:ASN:N	2.28	0.49
1:D:1129:ARG:HD2	1:D:1155:ASP:C	2.33	0.49
1:G:1845:MET:SD	1:G:1850:ALA:HB2	2.52	0.49
1:G:1900:TRP:CZ2	1:G:1937:ARG:NE	2.80	0.49
1:G:1963:ALA:HA	1:G:1988:THR:OG1	2.12	0.49
1:C:772:THR:O	1:C:773:HIS:CB	2.60	0.49
1:C:812:LEU:HD21	1:D:1061:HIS:HB2	1.94	0.49
1:G:1822:LEU:N	1:G:1823:PRO:HD2	2.27	0.49
1:G:1996:PHE:CZ	1:G:1999:PRO:HD2	2.47	0.49
1:D:991:ALA:CB	1:F:1629:ARG:NH2	2.66	0.49
1:D:1104:ILE:HG23	1:D:1104:ILE:O	2.13	0.49
1:G:2010:GLY:HA3	1:G:2023:TYR:HB3	1.94	0.49
1:A:13:PRO:HB2	1:A:199:PRO:HD3	1.95	0.48
1:C:691:ALA:CB	1:E:1329:ARG:NH1	2.75	0.48
1:C:761:HIS:HB2	1:D:1112:LEU:HD21	1.95	0.48
1:D:970:HIS:HA	2:D:317:HOH:O	2.13	0.48
1:E:1277:LEU:HD22	1:E:1297:GLY:CA	2.43	0.48
1:H:2186:ARG:O	1:H:2199:GLY:HA2	2.13	0.48
1:B:548:GLU:OE2	1:C:625:ILE:HG22	2.14	0.48
1:C:608:ASP:HB3	1:C:638:ASN:HD22	1.78	0.48
1:G:1826:ARG:N	1:G:1827:PRO:CD	2.76	0.48
1:H:2136:MET:HB3	1:H:2139:SER:OG	2.12	0.48
1:C:817:THR:HB	1:C:819:ARG:NH1	2.27	0.48
1:D:1097:THR:HA	1:D:1131:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1554:LEU:HD11	1:F:1582:TYR:HD2	1.78	0.48
1:H:2307:ALA:O	1:H:2311:PRO:HD2	2.14	0.48
1:H:2122:LEU:N	1:H:2123:PRO:HD2	2.28	0.48
1:H:2191:ALA:O	1:H:2192:ASP:C	2.51	0.48
1:D:947:ARG:HA	1:D:976:MET:HE1	1.95	0.48
1:D:1069:VAL:C	1:D:1070:ILE:HD12	2.34	0.48
1:E:1412:LEU:HD22	1:E:1416:LEU:HD12	1.95	0.48
1:D:1082:ARG:HH11	1:D:1082:ARG:CB	2.26	0.48
1:F:1702:SER:HB2	1:F:1706:SER:O	2.13	0.48
1:C:691:ALA:HB3	1:E:1329:ARG:NH2	2.29	0.48
1:F:1565:ASN:HB2	1:F:1648:HIS:CE1	2.49	0.48
1:B:466:VAL:HG12	1:B:468:ALA:H	1.78	0.47
1:B:548:GLU:OE2	1:C:625:ILE:CG2	2.62	0.47
1:F:1723:TYR:N	1:F:1723:TYR:CD2	2.82	0.47
1:G:2004:ILE:HG23	1:G:2004:ILE:O	2.14	0.47
1:B:496:PHE:CD1	1:B:496:PHE:C	2.86	0.47
1:A:232:LEU:HD23	1:A:232:LEU:C	2.35	0.47
1:C:811:PRO:HG3	1:C:823:TYR:CD1	2.50	0.47
1:D:1070:ILE:CG2	1:D:1094:ALA:HB2	2.44	0.47
1:F:1508:ASP:HB3	1:F:1538:ASN:HD22	1.79	0.47
1:H:2239:ASP:OD2	1:H:2239:ASP:N	2.46	0.47
1:C:748:HIS:CE1	1:C:773:HIS:CD2	3.02	0.47
1:C:775:HIS:CD2	1:C:804:ILE:HG12	2.50	0.47
1:E:1318:ARG:HD2	1:E:1327:PRO:CD	2.45	0.47
1:F:1588:LEU:HD13	1:F:1600:TRP:HD1	1.79	0.47
1:A:155:LYS:HD3	1:A:192:THR:O	2.14	0.47
1:A:230:ALA:H	1:A:254:GLU:CG	2.27	0.47
1:B:538:HIS:HD2	1:C:620:ASN:O	1.97	0.47
1:C:626:ARG:N	1:C:627:PRO:CD	2.78	0.47
1:C:782:ARG:CD	1:C:784:LEU:HD23	2.44	0.47
1:E:1313:VAL:HG13	1:E:1345:VAL:HG13	1.96	0.47
1:G:1810:PHE:HB2	1:G:1996:PHE:HE2	1.78	0.47
1:A:27:PRO:CA	1:D:928:GLN:HE22	2.26	0.47
1:C:622:LEU:N	1:C:623:PRO:HD2	2.30	0.47
1:E:1226:ARG:N	1:E:1227:PRO:CD	2.78	0.47
1:D:1029:ARG:HD3	1:F:1592:ASP:OD1	2.15	0.47
1:E:1217:VAL:HG11	1:E:1430:ALA:HB3	1.97	0.47
1:G:1871:LYS:HG2	1:G:1872:ASP:H	1.80	0.47
1:G:1911:THR:HG21	1:G:1940:LEU:HD22	1.97	0.47
1:C:615:ARG:HD2	2:C:167:HOH:O	2.13	0.47
1:C:755:LYS:HD3	1:C:792:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1868:TRP:HA	1:G:1873:ILE:CD1	2.39	0.47
1:E:1263:LEU:HD12	1:E:1286:ARG:HB3	1.95	0.47
1:G:1967:ALA:HB2	1:G:2042:GLY:O	2.15	0.47
1:D:995:THR:HG22	1:E:1419:ARG:NH1	2.29	0.47
1:H:2218:ARG:HD2	1:H:2227:PRO:CD	2.44	0.47
1:A:192:THR:HG21	1:B:476:VAL:HG21	1.97	0.46
1:D:991:ALA:HB2	1:D:1025:ASP:CG	2.35	0.46
1:G:1803:VAL:CG2	1:G:2039:PHE:CE2	2.98	0.46
1:C:667:ALA:O	1:C:673:ILE:HG21	2.15	0.46
1:C:776:VAL:HG21	1:D:1092:THR:HG21	1.97	0.46
1:C:790:TYR:OH	1:C:792:THR:HG22	2.15	0.46
1:E:1248:ASP:HA	1:E:1251:ARG:NH1	2.30	0.46
1:E:1348:HIS:CE1	1:E:1373:HIS:CD2	3.03	0.46
1:E:1348:HIS:HE1	1:E:1373:HIS:HD2	1.63	0.46
1:F:1670:ILE:CG2	1:F:1694:ALA:HB2	2.45	0.46
1:F:1682:ARG:HG2	1:F:1683:ILE:N	2.31	0.46
1:B:336:MET:HB3	1:B:339:SER:OG	2.14	0.46
1:B:346:HIS:CD2	1:B:348:ASP:HB2	2.50	0.46
1:E:1263:LEU:HD13	1:E:1267:ALA:HB1	1.96	0.46
1:E:1394:ALA:O	1:E:1433:ASN:HB3	2.15	0.46
1:F:1668:ALA:HB1	1:F:1670:ILE:CD1	2.45	0.46
1:F:1704:ILE:O	1:F:1704:ILE:HG23	2.15	0.46
1:G:1913:VAL:CG1	1:G:1931:MET:HE1	2.45	0.46
1:G:1999:PRO:CG	1:G:2026:ALA:HB3	2.44	0.46
1:A:71:LYS:O	1:A:75:PRO:HD2	2.16	0.46
1:B:507:ALA:O	1:B:511:PRO:HD2	2.16	0.46
1:F:1613:VAL:HG21	1:F:1631:MET:CE	2.45	0.46
1:F:1551:ARG:HH11	1:F:1551:ARG:HB3	1.79	0.46
1:F:1618:ARG:HD3	2:F:210:HOH:O	2.15	0.46
1:H:2280:ASP:O	1:H:2281:THR:C	2.53	0.46
1:D:1031:MET:O	1:D:1035:LEU:HG	2.14	0.46
1:G:1845:MET:CE	1:G:1863:LEU:HD21	2.45	0.46
1:G:1990:TYR:CD1	1:G:1990:TYR:C	2.89	0.46
1:A:175:HIS:CD2	1:A:204:ILE:HG12	2.50	0.46
1:A:175:HIS:HD2	1:A:204:ILE:O	1.98	0.46
1:C:690:TYR:HB3	1:C:695:THR:HG21	1.98	0.46
1:C:782:ARG:HD3	1:C:783:ILE:C	2.36	0.46
1:F:1634:LEU:O	1:F:1640:LEU:HD11	2.16	0.46
1:B:318:LEU:O	1:B:322:LEU:HB2	2.15	0.46
1:D:1022:GLU:OE1	1:E:1414:ARG:NH2	2.49	0.46
1:D:1123:TYR:N	1:D:1123:TYR:CD2	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1848:ASP:HA	1:G:1851:ARG:HH12	1.80	0.46
1:B:390:TYR:HB3	1:B:395:THR:HG21	1.97	0.46
1:C:770:ILE:HD12	1:C:770:ILE:N	2.31	0.46
1:E:1237:GLU:CG	1:E:1238:ASN:ND2	2.78	0.46
1:E:1380:ASP:O	1:E:1381:THR:C	2.54	0.46
1:F:1518:LEU:O	1:F:1522:LEU:HB2	2.15	0.46
1:F:1536:MET:HG3	1:F:1561:LEU:HG	1.98	0.46
1:G:1831:PHE:CD1	1:G:1910:LEU:HD23	2.51	0.45
1:G:2011:PRO:HD3	1:G:2023:TYR:HB3	1.98	0.45
1:A:76:MET:HE3	1:A:82:TYR:CD2	2.51	0.45
1:C:637:GLU:OE2	1:C:638:ASN:ND2	2.48	0.45
1:C:771:GLY:O	1:C:793:ASP:HA	2.16	0.45
1:F:1519:GLN:OE1	1:F:1552:GLY:HA3	2.16	0.45
1:B:326:ARG:N	1:B:327:PRO:CD	2.80	0.45
1:E:1267:ALA:O	1:E:1273:ILE:HG21	2.16	0.45
1:E:1430:ALA:O	1:E:1454:GLU:HG2	2.15	0.45
1:F:1510:PHE:HB2	1:F:1696:PHE:CE2	2.52	0.45
1:B:395:THR:HA	1:B:396:PRO:HD3	1.86	0.45
1:B:530:ALA:H	1:B:554:GLU:HG2	1.80	0.45
1:F:1565:ASN:HD22	1:F:1621:MET:CE	2.30	0.45
1:A:204:ILE:O	1:A:204:ILE:HG23	2.16	0.45
1:C:811:PRO:HD3	1:C:823:TYR:HB3	1.99	0.45
1:E:1400:HIS:CE1	1:E:1453:ILE:HD12	2.51	0.45
1:F:1587:PRO:HB2	1:F:1590:TYR:CD2	2.52	0.45
1:A:25:ILE:CG2	1:D:1148:GLU:OE2	2.65	0.45
1:E:1218:LEU:O	1:E:1218:LEU:HD22	2.17	0.45
1:G:2048:GLU:HG3	1:G:2048:GLU:O	2.17	0.45
1:H:2182:TYR:HD1	1:H:2182:TYR:H	1.64	0.45
1:B:470:ILE:HD12	1:B:470:ILE:N	2.31	0.45
1:C:668:TRP:CD2	1:F:1719:ARG:HD2	2.51	0.45
1:C:792:THR:OG1	1:D:1076:VAL:HG11	2.16	0.45
1:D:986:ARG:O	1:D:999:GLY:HA2	2.17	0.45
1:D:1015:LEU:HG	1:D:1031:MET:HE3	1.97	0.45
1:G:1837:GLU:OE1	1:G:1865:ASN:HB3	2.16	0.45
1:G:1864:GLY:O	1:G:1867:ALA:N	2.47	0.45
1:G:2003:ILE:HD11	1:G:2008:ILE:HG23	1.99	0.45
1:E:1396:PHE:CD1	1:E:1396:PHE:C	2.88	0.45
1:F:1711:PRO:HG3	1:F:1723:TYR:CD1	2.52	0.45
1:G:1918:ARG:HD2	1:G:1927:PRO:CD	2.46	0.45
1:A:102:THR:HG22	1:A:111:THR:OG1	2.17	0.45
1:A:203:ILE:HD13	1:B:457:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:792:THR:HG21	1:D:1076:VAL:HG21	1.98	0.45
1:D:1127:GLU:O	1:D:1127:GLU:CD	2.55	0.45
1:E:1274:TYR:N	1:E:1275:PRO:HD2	2.32	0.45
1:H:2136:MET:O	1:H:2139:SER:OG	2.35	0.45
1:H:2245:VAL:HG21	1:H:2262:LEU:HD23	1.97	0.45
1:A:119:VAL:HG23	1:A:154:GLU:OE1	2.16	0.45
1:B:482:ARG:HG2	1:B:483:ILE:H	1.82	0.45
1:G:1889:ASN:OD1	1:G:1889:ASN:N	2.49	0.45
1:G:1892:ASP:HB3	1:G:1895:THR:HG23	1.98	0.45
1:G:1970:ILE:N	1:G:1970:ILE:CD1	2.80	0.44
1:H:2282:ARG:CG	1:H:2283:ILE:H	2.30	0.44
1:B:490:TYR:HH	1:B:492:THR:HG22	1.81	0.44
1:F:1613:VAL:HG21	1:F:1631:MET:HE1	1.99	0.44
1:F:1732:LEU:C	1:F:1732:LEU:HD23	2.38	0.44
1:A:182:ARG:HD2	1:A:184:LEU:HD23	1.99	0.44
1:B:449:ALA:O	1:B:455:LYS:HE3	2.18	0.44
1:C:815:PHE:HB3	1:D:1028:PHE:CD2	2.53	0.44
1:H:2164:GLY:HA2	1:H:2187:PRO:HG3	1.99	0.44
1:H:2304:ILE:O	1:H:2304:ILE:HG23	2.17	0.44
1:A:207:ALA:O	1:A:211:PRO:HD2	2.18	0.44
1:B:337:GLU:OE2	1:B:448:HIS:CE1	2.70	0.44
1:C:692:ASP:HA	1:C:693:PRO:HD3	1.86	0.44
1:C:782:ARG:CG	1:C:783:ILE:N	2.80	0.44
1:C:823:TYR:HD2	1:C:823:TYR:O	2.01	0.44
1:E:1348:HIS:CE1	1:E:1373:HIS:HB2	2.53	0.44
1:E:1369:VAL:C	1:E:1370:ILE:HD12	2.37	0.44
1:G:1861:LEU:N	1:G:1861:LEU:CD2	2.76	0.44
1:B:482:ARG:HD3	1:B:483:ILE:O	2.17	0.44
1:D:1148:GLU:O	1:D:1148:GLU:HG3	2.18	0.44
1:H:2291:GLN:NE2	1:H:2294:ALA:HA	2.32	0.44
1:D:926:ARG:HB3	1:D:927:PRO:HD3	2.00	0.44
1:D:1055:LYS:HD2	2:D:146:HOH:O	2.17	0.44
1:E:1217:VAL:CG1	1:E:1430:ALA:HB3	2.47	0.44
1:E:1309:LYS:HE3	1:E:1309:LYS:HB2	1.85	0.44
1:E:1382:ARG:CB	1:E:1382:ARG:NH1	2.76	0.44
1:E:1415:PHE:HB3	1:F:1628:PHE:CE2	2.52	0.44
1:G:1878:SER:C	1:G:1880:ASP:H	2.21	0.44
1:H:2331:GLU:HB2	1:H:2353:ILE:HD13	1.99	0.44
1:A:79:GLU:HG2	1:A:79:GLU:H	1.62	0.44
1:B:443:VAL:O	1:B:466:VAL:HG13	2.17	0.44
1:C:803:ILE:O	1:C:804:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1547:ARG:HA	1:F:1576:MET:CE	2.41	0.44
1:G:1877:LEU:HD22	1:G:1897:GLY:HA3	2.00	0.44
1:G:1892:ASP:HA	1:G:1893:PRO:HD3	1.82	0.44
1:H:2182:TYR:N	1:H:2182:TYR:CD1	2.86	0.44
1:B:387:PRO:HB2	1:B:390:TYR:CE2	2.53	0.44
1:D:908:ASP:HB3	1:D:938:ASN:HD22	1.83	0.44
1:E:1370:ILE:HD12	1:E:1370:ILE:N	2.33	0.44
1:B:510:GLY:HA3	1:B:523:TYR:HB3	2.00	0.44
1:G:1870:HIS:H	1:G:1873:ILE:HD12	1.83	0.44
1:E:1218:LEU:C	1:E:1218:LEU:HD13	2.38	0.43
1:F:1585:VAL:HG12	1:F:1614:ASN:HB2	2.00	0.43
1:H:2191:ALA:HB2	1:H:2225:ASP:OD2	2.17	0.43
1:B:387:PRO:HB2	1:B:390:TYR:CD2	2.53	0.43
1:F:1526:ARG:N	1:F:1527:PRO:CD	2.81	0.43
1:F:1644:PHE:CD1	1:F:1644:PHE:C	2.92	0.43
1:G:1836:MET:HB3	1:G:1839:SER:HG	1.83	0.43
1:G:1946:ASP:C	1:G:1946:ASP:OD2	2.55	0.43
1:A:8:ASP:OD1	1:A:172:THR:HB	2.17	0.43
1:A:92:ASP:HA	1:A:93:PRO:HD3	1.84	0.43
1:B:392:ASP:HB3	1:B:395:THR:HG23	1.99	0.43
1:C:617:VAL:HG13	1:C:854:GLU:OE2	2.18	0.43
1:C:718:ARG:HD2	1:C:727:PRO:HD2	2.00	0.43
1:E:1221:HIS:CE1	1:E:1450:TYR:OH	2.72	0.43
1:F:1660:TRP:CH2	1:F:1684:LEU:HD22	2.54	0.43
1:G:1982:ARG:HG2	1:G:1983:ILE:N	2.33	0.43
1:H:2282:ARG:HG2	1:H:2283:ILE:H	1.82	0.43
1:E:1310:LEU:HD12	1:E:1342:THR:O	2.18	0.43
1:G:1864:GLY:O	1:G:1865:ASN:C	2.57	0.43
1:G:2017:THR:O	1:G:2018:GLU:HB2	2.19	0.43
1:D:972:ASP:O	1:D:975:PRO:HG2	2.18	0.43
1:D:1029:ARG:NH1	1:F:1592:ASP:N	2.66	0.43
1:D:1111:PRO:CD	1:D:1123:TYR:HD1	2.32	0.43
1:H:2192:ASP:HB3	1:H:2195:THR:CG2	2.42	0.43
1:A:147:PHE:O	1:A:171:GLY:HA2	2.19	0.43
1:E:1221:HIS:C	1:E:1223:PRO:HD2	2.39	0.43
1:E:1319:VAL:HG12	1:E:1320:PHE:CD2	2.54	0.43
1:B:336:MET:HG3	1:B:361:LEU:HG	2.01	0.43
1:C:811:PRO:O	1:C:814:ARG:HB2	2.19	0.43
1:E:1264:GLY:HA2	1:E:1287:PRO:HG3	2.00	0.43
1:G:1884:ILE:HG22	1:G:1885:VAL:N	2.34	0.43
1:D:1082:ARG:HD3	1:D:1083:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:HIS:O	1:B:373:ILE:HD12	2.18	0.43
1:C:695:THR:HA	1:C:696:PRO:HD3	1.88	0.43
1:E:1417:THR:O	1:E:1418:GLU:HB2	2.18	0.43
1:F:1503:VAL:HG21	1:F:1739:PHE:CE2	2.54	0.43
1:G:1999:PRO:CB	1:G:2026:ALA:HB3	2.48	0.43
1:C:715:LEU:HB3	1:C:747:PHE:HD1	1.84	0.42
1:D:1117:THR:HB	1:D:1119:ARG:NH1	2.34	0.42
1:E:1348:HIS:CE1	1:E:1373:HIS:HD2	2.37	0.42
1:G:1902:THR:HG22	1:G:1911:THR:CG2	2.49	0.42
1:A:37:GLU:OE2	1:A:148:HIS:CE1	2.72	0.42
1:G:1808:ASP:OD1	1:G:1972:THR:HB	2.19	0.42
1:A:118:ARG:HD2	1:A:127:PRO:HD3	2.00	0.42
1:E:1236:MET:HE2	1:E:1253:ALA:HB2	1.99	0.42
1:E:1378:THR:HA	1:F:1678:THR:HA	2.01	0.42
1:G:1822:LEU:HD21	1:G:1832:VAL:HG11	2.01	0.42
1:G:1865:ASN:N	1:G:1916:LEU:HD21	2.34	0.42
1:G:1895:THR:HA	1:G:1896:PRO:HD3	1.90	0.42
1:H:2122:LEU:O	1:H:2122:LEU:HD22	2.19	0.42
1:H:2219:VAL:O	1:H:2221:MET:HG3	2.19	0.42
1:D:1013:VAL:HG11	1:D:1045:VAL:HG22	2.01	0.42
1:F:1551:ARG:HH11	1:F:1551:ARG:CB	2.32	0.42
1:H:2275:HIS:HA	1:H:2296:PHE:HB3	2.01	0.42
1:H:2317:THR:HB	1:H:2319:ARG:CZ	2.49	0.42
1:D:1048:HIS:CE1	1:D:1073:HIS:HD2	2.37	0.42
1:B:389:ASN:O	1:B:425:ASP:HB2	2.20	0.42
1:B:533:ASN:OD1	1:B:551:ARG:HG3	2.20	0.42
1:F:1739:PHE:HD1	1:F:1744:ALA:HA	1.84	0.42
1:G:1968:ALA:HB1	1:G:1970:ILE:HD13	2.02	0.42
1:G:1970:ILE:HG21	1:G:1994:ALA:HB2	2.02	0.42
1:A:196:PHE:CD1	1:A:196:PHE:C	2.92	0.42
1:B:364:GLY:HA2	1:B:387:PRO:HG3	2.01	0.42
1:C:608:ASP:O	1:C:796:PHE:HB2	2.19	0.42
1:A:149:ALA:O	1:A:155:LYS:HE3	2.19	0.42
1:A:157:ALA:HB2	1:B:503:ILE:HD13	2.02	0.42
1:B:539:PHE:HA	1:B:543:LYS:O	2.19	0.42
1:C:811:PRO:HD3	1:C:823:TYR:CB	2.49	0.42
1:D:922:LEU:N	1:D:923:PRO:HD2	2.33	0.42
1:F:1682:ARG:CG	1:F:1683:ILE:N	2.83	0.42
1:G:1887:PRO:HB3	1:G:1916:LEU:HG	2.01	0.42
1:G:1918:ARG:HD2	1:G:1927:PRO:HD3	2.02	0.42
1:A:86:ARG:HB2	1:A:87:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1215:ARG:NH2	2:E:9:HOH:O	2.51	0.42
1:F:1675:HIS:CD2	1:F:1704:ILE:HG12	2.54	0.42
1:F:1751:ARG:NH1	1:F:1753:ILE:HD11	2.34	0.42
1:G:1863:LEU:C	1:G:1914:ASN:HD21	2.22	0.42
1:C:676:MET:HE2	1:C:682:TYR:CD1	2.55	0.42
1:D:1039:ASP:OD2	1:D:1039:ASP:N	2.48	0.42
1:G:1805:PHE:O	1:G:2034:GLY:HA3	2.20	0.42
1:G:1952:THR:HG21	1:H:2274:THR:HB	2.02	0.42
1:H:2126:ARG:N	1:H:2127:PRO:CD	2.83	0.41
1:C:692:ASP:N	1:E:1329:ARG:HH11	2.15	0.41
1:C:768:ALA:HB1	1:C:770:ILE:CD1	2.50	0.41
1:E:1208:ASP:HB2	1:E:1396:PHE:HB2	2.01	0.41
1:F:1613:VAL:HG13	1:F:1645:VAL:HG22	2.02	0.41
1:F:1615:LEU:HB3	1:F:1647:PHE:HD1	1.85	0.41
1:A:15:ARG:NH2	2:A:256:HOH:O	2.51	0.41
1:A:113:VAL:CG1	1:A:145:VAL:HG22	2.49	0.41
1:E:1226:ARG:O	1:E:1226:ARG:HD3	2.20	0.41
1:A:180:ASP:O	1:A:181:THR:C	2.59	0.41
1:D:1151:ARG:NE	1:D:1153:ILE:HD11	2.35	0.41
1:H:2209:LYS:HE3	1:H:2209:LYS:HB2	1.95	0.41
1:D:964:GLY:O	1:D:965:ASN:C	2.59	0.41
1:D:964:GLY:O	1:D:967:ALA:HB2	2.21	0.41
1:F:1586:ARG:O	1:F:1599:GLY:HA2	2.20	0.41
1:H:2246:ASP:C	1:H:2246:ASP:OD2	2.58	0.41
1:A:36:MET:HB3	1:A:39:SER:OG	2.21	0.41
1:B:346:HIS:CD2	1:B:349:ALA:H	2.38	0.41
1:D:918:LEU:HD13	1:D:918:LEU:C	2.41	0.41
1:D:936:MET:HE2	1:D:953:ALA:HB2	2.02	0.41
1:G:1890:TYR:HB3	1:G:1895:THR:HG21	2.02	0.41
1:H:2143:PHE:HD1	1:H:2166:HIS:CD2	2.38	0.41
1:F:1564:GLY:HA2	1:F:1587:PRO:HG3	2.01	0.41
1:G:1810:PHE:CB	1:G:1996:PHE:CE2	3.03	0.41
1:G:1837:GLU:HG3	1:G:1866:HIS:HB2	2.02	0.41
1:H:2294:ALA:O	1:H:2333:ASN:HB3	2.21	0.41
1:D:995:THR:HA	1:D:996:PRO:HD3	1.78	0.41
1:F:1671:GLY:HA3	1:F:1692:THR:O	2.21	0.41
1:H:2269:VAL:C	1:H:2270:ILE:HD12	2.41	0.41
1:H:2299:PRO:HG2	1:H:2305:GLY:HA2	2.03	0.41
1:A:36:MET:HE1	1:A:53:ALA:HB2	2.03	0.41
1:B:502:SER:HB2	1:B:506:SER:O	2.21	0.41
1:C:804:ILE:HG12	1:C:804:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1099:PRO:HB2	1:D:1126:ALA:HB3	2.02	0.41
1:D:1127:GLU:HG3	2:D:230:HOH:O	2.21	0.41
1:E:1292:ASP:HB3	1:E:1295:THR:CG2	2.43	0.41
1:E:1313:VAL:CG1	1:E:1345:VAL:HG22	2.50	0.41
1:F:1680:ASP:O	1:F:1681:THR:C	2.59	0.41
1:G:1944:PHE:CD2	1:G:1968:ALA:HB3	2.56	0.41
1:B:415:LEU:HD11	1:B:431:MET:CG	2.48	0.41
1:C:739:ASP:OD2	1:C:739:ASP:N	2.54	0.41
1:F:1536:MET:HB3	1:F:1539:SER:OG	2.20	0.41
1:H:2154:LEU:HD11	1:H:2182:TYR:CD2	2.55	0.41
1:C:715:LEU:HB3	1:C:747:PHE:CD1	2.56	0.40
1:H:2277:PRO:HA	1:H:2293:ASP:O	2.21	0.40
1:B:511:PRO:HG3	1:B:523:TYR:HD1	1.86	0.40
1:B:548:GLU:CD	1:C:625:ILE:CG2	2.89	0.40
1:E:1360:TRP:CH2	1:E:1384:LEU:HD22	2.55	0.40
1:G:1902:THR:HG22	1:G:1911:THR:HG23	2.02	0.40
1:B:365:ASN:HB2	1:B:448:HIS:CE1	2.56	0.40
1:C:782:ARG:HD3	1:C:783:ILE:O	2.21	0.40
1:F:1507:GLY:HA3	1:F:1695:GLY:O	2.22	0.40
1:G:1834:VAL:O	1:G:1861:LEU:HA	2.21	0.40
1:H:2118:LEU:C	1:H:2118:LEU:HD13	2.42	0.40
1:H:2303:ILE:CD1	1:H:2311:PRO:HB2	2.51	0.40
1:E:1295:THR:HA	1:E:1296:PRO:HD3	1.90	0.40
1:H:2219:VAL:HG12	1:H:2220:PHE:CG	2.56	0.40
1:H:2302:SER:HB3	1:H:2326:ALA:CB	2.52	0.40
1:H:2323:TYR:HD2	1:H:2323:TYR:O	2.04	0.40
1:C:734:LEU:C	1:C:736:GLU:H	2.25	0.40
1:D:1107:ALA:O	1:D:1111:PRO:HD2	2.21	0.40
1:F:1717:THR:HB	1:F:1719:ARG:NH1	2.36	0.40
1:G:1803:VAL:HG23	1:G:1803:VAL:O	2.21	0.40
1:G:1831:PHE:CE2	1:G:1859:GLY:HA3	2.56	0.40
1:G:1967:ALA:HB1	1:G:2039:PHE:CD1	2.56	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	253/255 (99%)	236 (93%)	13 (5%)	4 (2%)	9	9
1	B	253/255 (99%)	234 (92%)	15 (6%)	4 (2%)	9	9
1	C	253/255 (99%)	238 (94%)	12 (5%)	3 (1%)	13	14
1	D	253/255 (99%)	235 (93%)	13 (5%)	5 (2%)	7	6
1	E	253/255 (99%)	228 (90%)	21 (8%)	4 (2%)	9	9
1	F	253/255 (99%)	236 (93%)	14 (6%)	3 (1%)	13	14
1	G	253/255 (99%)	206 (81%)	36 (14%)	11 (4%)	2	1
1	H	253/255 (99%)	229 (90%)	17 (7%)	7 (3%)	5	3
All	All	2024/2040 (99%)	1842 (91%)	141 (7%)	41 (2%)	7	6

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	ASP
1	D	965	ASN
1	G	1880	ASP
1	B	473	HIS
1	C	608	ASP
1	E	1208	ASP
1	F	1508	ASP
1	F	1704	ILE
1	G	1808	ASP
1	G	1872	ASP
1	G	1973	HIS
1	H	2171	LYS
1	B	308	ASP
1	C	735	LEU
1	C	773	HIS
1	D	908	ASP
1	E	1373	HIS
1	F	1673	HIS
1	G	1865	ASN
1	H	2239	ASP
1	H	2273	HIS
1	H	2304	ILE
1	A	8	ASP

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Mol	Chain	Res	Type
1	A	135	LEU
1	A	173	HIS
1	A	204	ILE
1	D	989	ASN
1	D	1073	HIS
1	E	1404	ILE
1	G	1889	ASN
1	G	1939	ASP
1	H	2235	LEU
1	B	405	VAL
1	D	1104	ILE
1	G	2004	ILE
1	H	2165	ASN
1	H	2310	GLY
1	E	1410	GLY
1	G	1841	GLY
1	G	1873	ILE
1	G	1905	VAL

5.3.2 Protein sidechains (i)

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	199/199 (100%)	181 (91%)	18 (9%)	9 11
1	B	199/199 (100%)	181 (91%)	18 (9%)	9 11
1	C	199/199 (100%)	179 (90%)	20 (10%)	7 9
1	D	199/199 (100%)	185 (93%)	14 (7%)	15 19
1	E	199/199 (100%)	181 (91%)	18 (9%)	9 11
1	F	199/199 (100%)	182 (92%)	17 (8%)	10 13
1	G	199/199 (100%)	185 (93%)	14 (7%)	15 19
1	H	199/199 (100%)	185 (93%)	14 (7%)	15 19
All	All	1592/1592 (100%)	1459 (92%)	133 (8%)	11 13

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	17	VAL
1	A	18	LEU
1	A	22	LEU
1	A	25	ILE
1	A	26	ARG
1	A	37	GLU
1	A	61	LEU
1	A	71	LYS
1	A	79	GLU
1	A	138	ASP
1	A	166	VAL
1	A	182	ARG
1	A	196	PHE
1	A	212	LEU
1	A	214	ARG
1	A	223	TYR
1	A	227	GLU
1	B	308	ASP
1	B	317	VAL
1	B	318	LEU
1	B	322	LEU
1	B	326	ARG
1	B	337	GLU
1	B	361	LEU
1	B	371	LYS
1	B	413	VAL
1	B	438	ASP
1	B	465	ARG
1	B	482	ARG
1	B	496	PHE
1	B	523	TYR
1	B	527	GLU
1	B	529	ARG
1	B	538	HIS
1	B	553	ILE
1	C	608	ASP
1	C	617	VAL
1	C	618	LEU
1	C	622	LEU
1	C	626	ARG
1	C	637	GLU
1	C	648	ASP

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Mol	Chain	Res	Type
1	C	661	LEU
1	C	671	LYS
1	C	702	THR
1	C	725	ASP
1	C	738	ASP
1	C	765	ARG
1	C	775	HIS
1	C	782	ARG
1	C	796	PHE
1	C	812	LEU
1	C	814	ARG
1	C	823	TYR
1	C	827	GLU
1	D	903	VAL
1	D	908	ASP
1	D	917	VAL
1	D	922	LEU
1	D	926	ARG
1	D	937	GLU
1	D	971	LYS
1	D	1038	ASP
1	D	1082	ARG
1	D	1096	PHE
1	D	1112	LEU
1	D	1123	TYR
1	D	1127	GLU
1	D	1129	ARG
1	E	1201	MET
1	E	1222	LEU
1	E	1226	ARG
1	E	1237	GLU
1	E	1246	HIS
1	E	1261	LEU
1	E	1271	LYS
1	E	1272	ASP
1	E	1298	VAL
1	E	1325	ASP
1	E	1338	ASP
1	E	1362	LEU
1	E	1382	ARG
1	E	1396	PHE
1	E	1412	LEU

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Mol	Chain	Res	Type
1	E	1423	TYR
1	E	1427	GLU
1	E	1429	ARG
1	F	1508	ASP
1	F	1518	LEU
1	F	1522	LEU
1	F	1526	ARG
1	F	1537	GLU
1	F	1561	LEU
1	F	1571	LYS
1	F	1613	VAL
1	F	1625	ASP
1	F	1638	ASP
1	F	1682	ARG
1	F	1696	PHE
1	F	1712	LEU
1	F	1714	ARG
1	F	1723	TYR
1	F	1727	GLU
1	F	1738	HIS
1	G	1808	ASP
1	G	1822	LEU
1	G	1846	HIS
1	G	1861	LEU
1	G	1871	LYS
1	G	1938	ASP
1	G	1947	PHE
1	G	1975	HIS
1	G	1982	ARG
1	G	2012	LEU
1	G	2014	ARG
1	G	2023	TYR
1	G	2027	GLU
1	G	2029	ARG
1	H	2108	ASP
1	H	2122	LEU
1	H	2126	ARG
1	H	2137	GLU
1	H	2139	SER
1	H	2161	LEU
1	H	2171	LYS
1	H	2238	ASP

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Mol	Chain	Res	Type
1	H	2282	ARG
1	H	2296	PHE
1	H	2314	ARG
1	H	2323	TYR
1	H	2327	GLU
1	H	2329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	28	GLN
1	A	38	ASN
1	A	46	HIS
1	A	69	HIS
1	A	114	ASN
1	A	148	HIS
1	A	173	HIS
1	A	175	HIS
1	B	319	GLN
1	B	321	HIS
1	B	328	GLN
1	B	338	ASN
1	B	366	HIS
1	B	414	ASN
1	B	448	HIS
1	B	473	HIS
1	B	475	HIS
1	B	538	HIS
1	C	621	HIS
1	C	628	GLN
1	C	638	ASN
1	C	646	HIS
1	C	669	HIS
1	C	748	HIS
1	C	761	HIS
1	C	773	HIS
1	C	775	HIS
1	D	921	HIS
1	D	928	GLN
1	D	938	ASN
1	D	946	HIS

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Mol	Chain	Res	Type
1	D	965	ASN
1	D	966	HIS
1	D	969	HIS
1	D	1014	ASN
1	D	1048	HIS
1	D	1061	HIS
1	D	1073	HIS
1	D	1075	HIS
1	E	1221	HIS
1	E	1228	GLN
1	E	1238	ASN
1	E	1246	HIS
1	E	1314	ASN
1	E	1348	HIS
1	E	1373	HIS
1	E	1375	HIS
1	F	1521	HIS
1	F	1538	ASN
1	F	1546	HIS
1	F	1565	ASN
1	F	1566	HIS
1	F	1569	HIS
1	F	1614	ASN
1	F	1648	HIS
1	F	1661	HIS
1	F	1673	HIS
1	F	1675	HIS
1	G	1821	HIS
1	G	1828	GLN
1	G	1838	ASN
1	G	1846	HIS
1	G	1866	HIS
1	G	1869	HIS
1	G	1973	HIS
1	H	2121	HIS
1	H	2128	GLN
1	H	2138	ASN
1	H	2146	HIS
1	H	2169	HIS
1	H	2214	ASN
1	H	2248	HIS
1	H	2275	HIS

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Mol	Chain	Res	Type
1	H	2321	HIS
1	H	2338	HIS

5.3.3 RNA (i)

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 monosaccharides 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 (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, 95th 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^2)	Q<0.9
1	A	255/255 (100%)	-0.11	1 (0%)	92	95	21, 31, 55, 92	0
1	B	255/255 (100%)	0.07	2 (0%)	86	89	22, 35, 69, 102	0
1	C	255/255 (100%)	0.05	4 (1%)	72	77	22, 33, 62, 93	0
1	D	255/255 (100%)	0.23	10 (3%)	39	46	22, 39, 72, 90	0
1	E	255/255 (100%)	0.38	8 (3%)	49	56	26, 44, 73, 102	0
1	F	255/255 (100%)	0.15	8 (3%)	49	56	24, 37, 68, 113	0
1	G	255/255 (100%)	0.72	18 (7%)	16	21	33, 55, 88, 109	0
1	H	255/255 (100%)	0.11	4 (1%)	72	77	25, 40, 70, 104	0
All	All	2040/2040 (100%)	0.20	55 (2%)	54	62	21, 39, 73, 113	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1305	VAL	4.0
1	H	2327	GLU	3.9
1	G	2023	TYR	3.7
1	G	1905	VAL	3.7
1	F	1638	ASP	3.6
1	E	1423	TYR	3.4
1	D	982	TYR	3.2
1	E	1282	TYR	3.2
1	G	1873	ILE	3.2
1	G	1831	PHE	3.1
1	E	1337	ARG	3.1
1	G	1874	TYR	3.1
1	G	1871	LYS	3.0
1	D	1092	THR	3.0
1	G	1940	LEU	3.0
1	G	1891	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	1639	ASP	2.9
1	D	948	ASP	2.9
1	G	1847	ARG	2.8
1	G	1933	ALA	2.7
1	G	1996	PHE	2.6
1	D	1039	ASP	2.6
1	F	1605	VAL	2.6
1	D	951	ARG	2.6
1	D	973	ILE	2.6
1	G	1882	TYR	2.5
1	D	971	LYS	2.5
1	H	2239	ASP	2.5
1	G	1960	TRP	2.4
1	E	1427	GLU	2.4
1	D	1123	TYR	2.4
1	G	1878	SER	2.4
1	B	438	ASP	2.4
1	H	2322	ARG	2.4
1	E	1338	ASP	2.3
1	G	1900	TRP	2.3
1	E	1273	ILE	2.3
1	B	522	ARG	2.3
1	F	1723	TYR	2.3
1	F	1748	GLU	2.2
1	D	1096	PHE	2.2
1	D	1006	ASN	2.1
1	C	705	VAL	2.1
1	C	673	ILE	2.1
1	F	1565	ASN	2.1
1	G	1937	ARG	2.1
1	F	1692	THR	2.1
1	G	1906	ASN	2.1
1	C	822	ARG	2.0
1	F	1573	ILE	2.0
1	C	691	ALA	2.0
1	A	223	TYR	2.0
1	E	1265	ASN	2.0
1	H	2323	TYR	2.0
1	G	2055	ASP	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 monosaccharides 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.