Full wwPDB X-ray Structure Validation Report (i)

Jan 22, 2018 – 08:27 PM EST

PDB ID	:	5I8I
Title	:	Crystal Structure of the K. lactis Urea Amidolyase
Authors	:	Zhao, J.; Xiang, S.
Deposited on	:	2016-02-19
Resolution	:	6.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

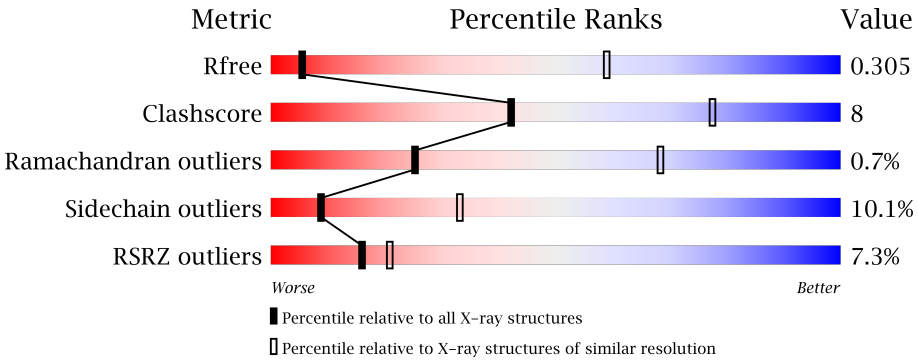
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 6.50 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	1098 (9.00-3.70)
Clashscore	112137	1031 (9.00-3.80)
Ramachandran outliers	110173	1000 (9.00-3.76)
Sidechain outliers	110143	1096 (9.00-3.70)
RSRZ outliers	101464	1000 (9.00-3.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	1829	7% 70% 18% • 9%
1	B	1829	5% 69% 17% • 9%
1	C	1829	8% 70% 17% • 9%
1	D	1829	6% 70% 17% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 51722 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.

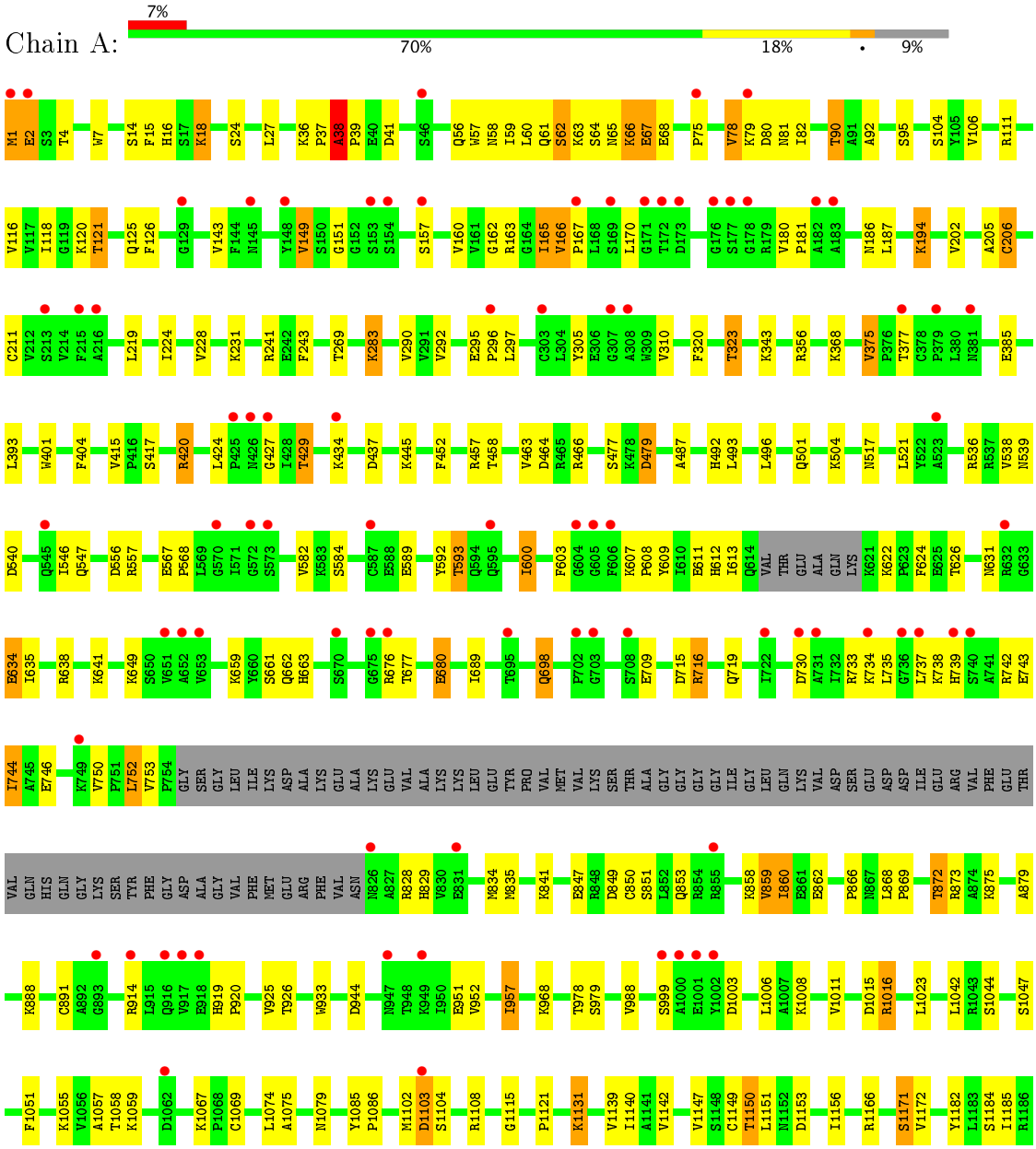
- Molecule 1 is a protein called Urea Amidolyase.

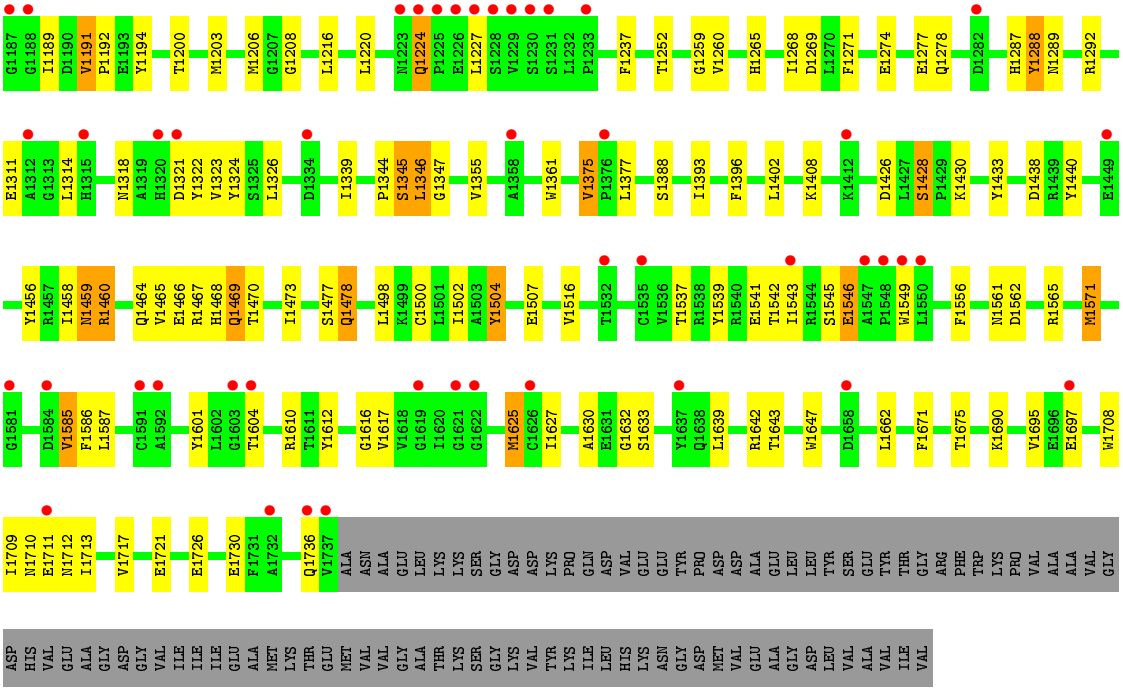
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0	0
			12939	8253	2183	2456	47			
1	B	1658	Total	C	N	O	S	0	0	0
			12922	8243	2181	2452	46			
1	C	1660	Total	C	N	O	S	0	0	0
			12939	8253	2183	2456	47			
1	D	1658	Total	C	N	O	S	0	0	0
			12922	8243	2181	2452	46			

3 Residue-property plots (i)

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.

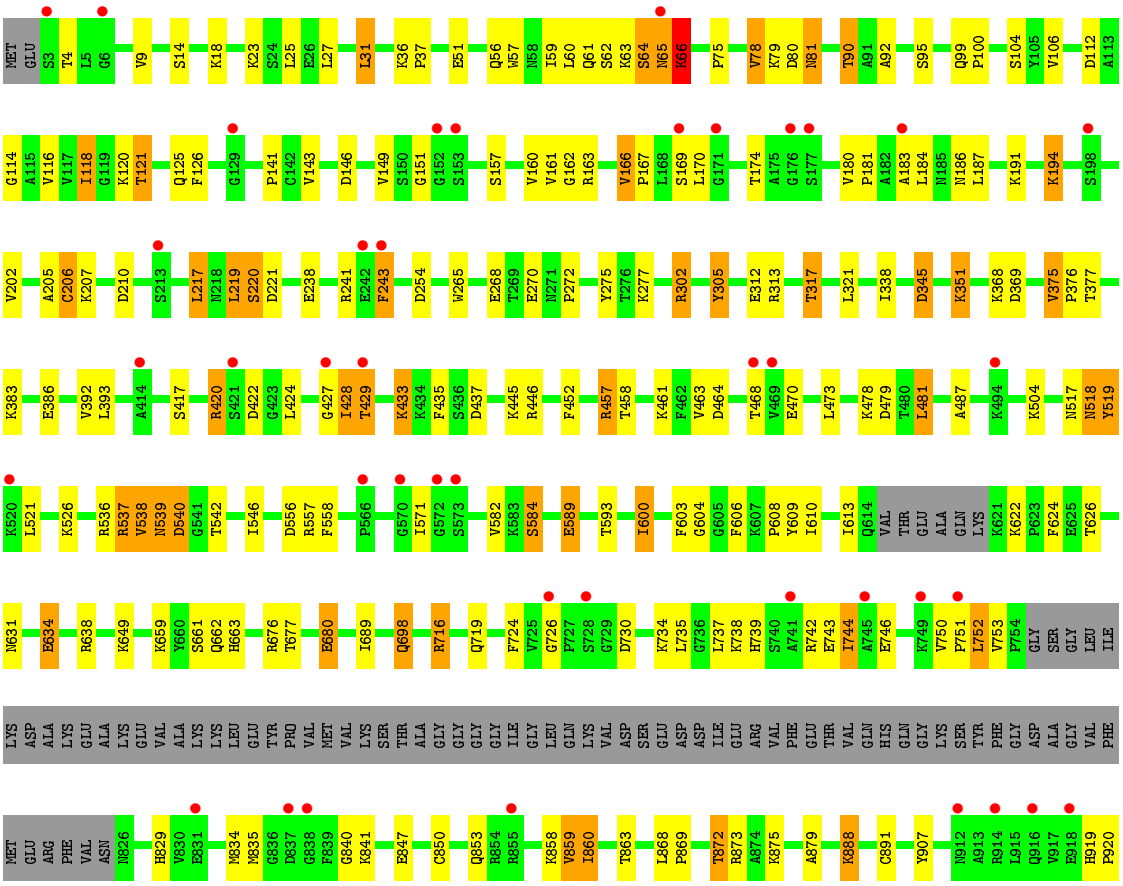
- Molecule 1: Urea Amidolyase

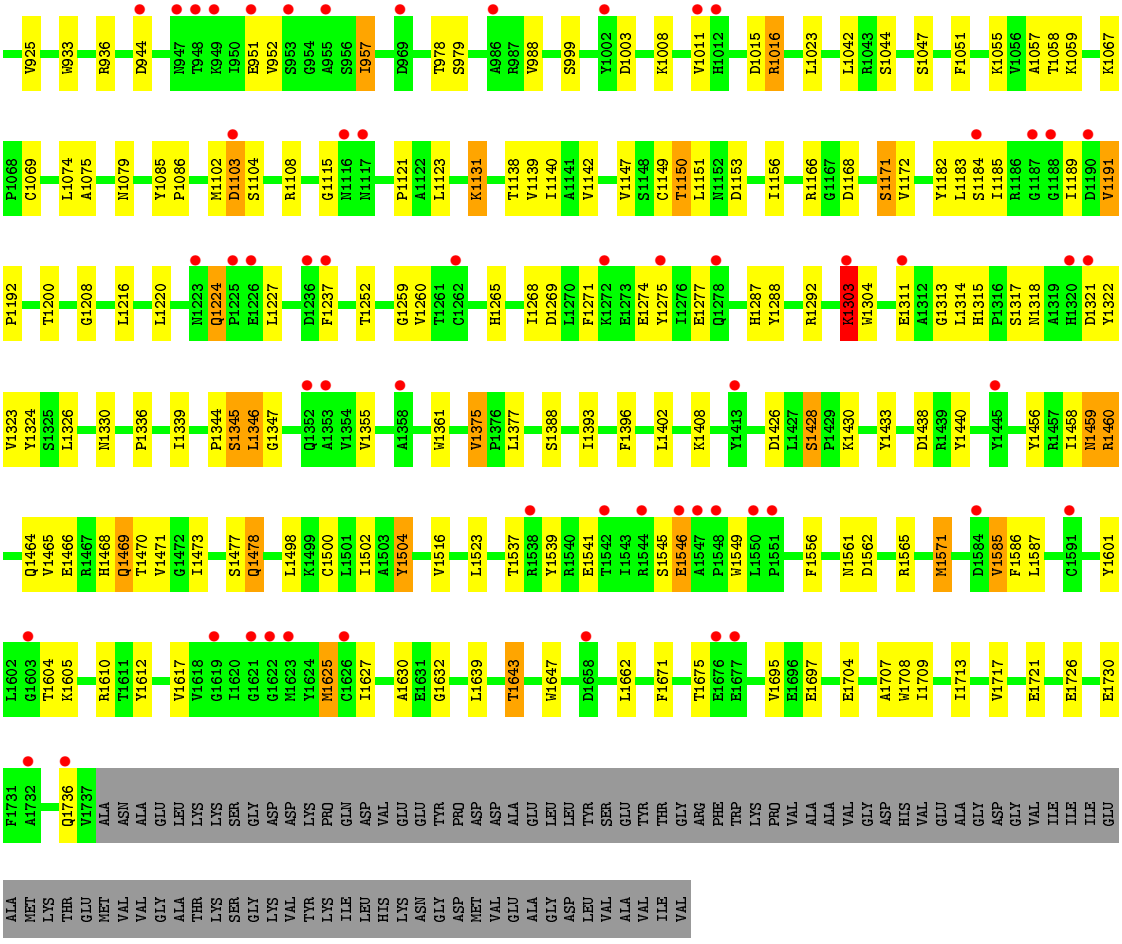




- Molecule 1: Urea Amidolyase

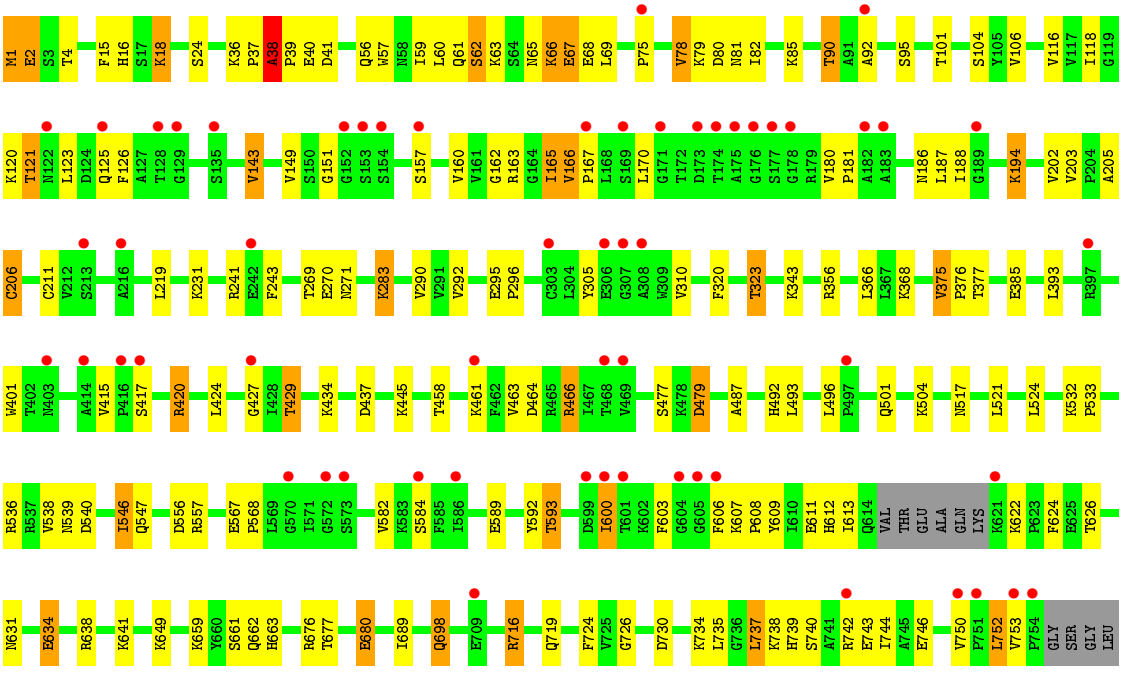
Chain B:

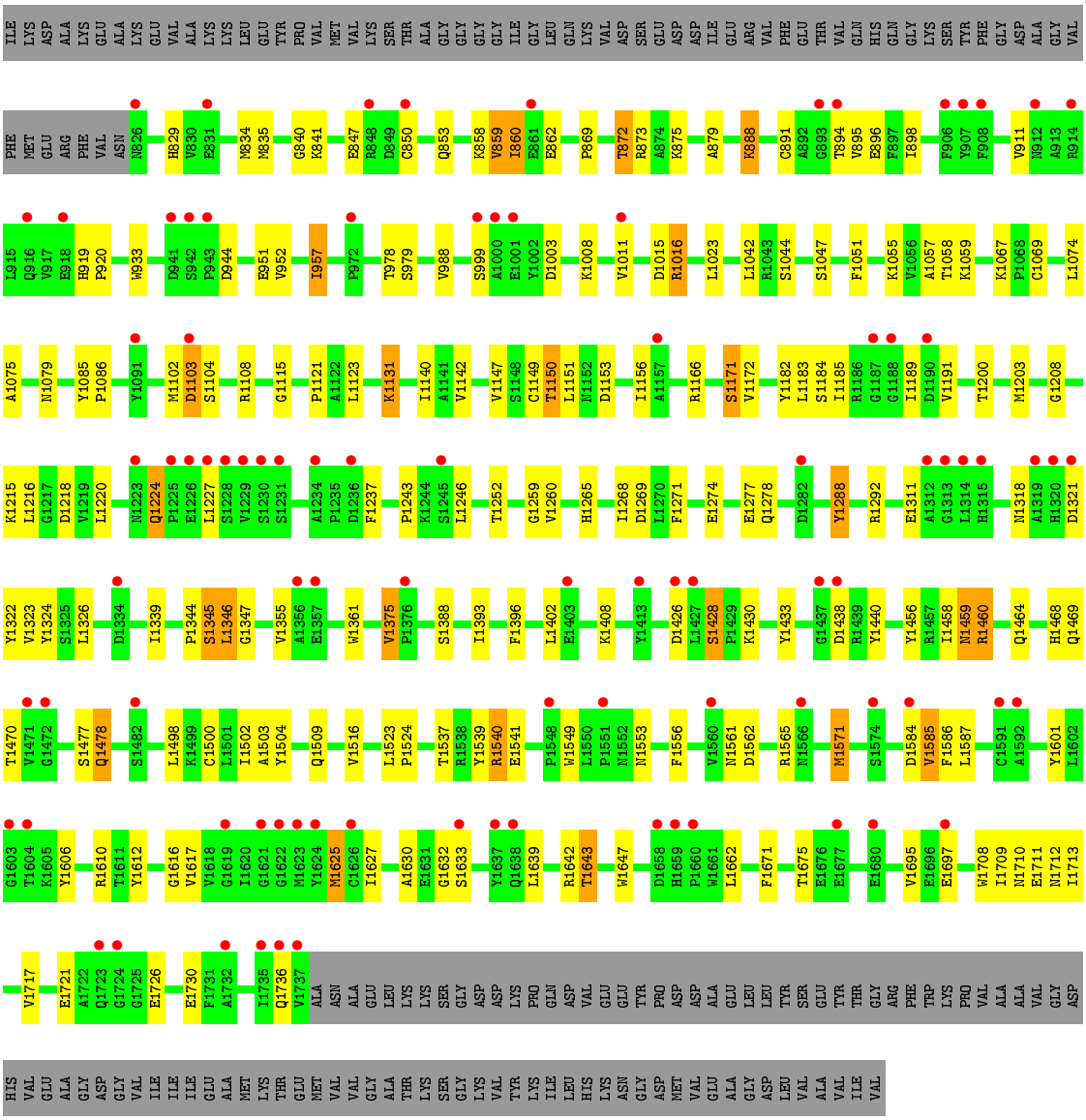




• Molecule 1: Urea Amidolyase

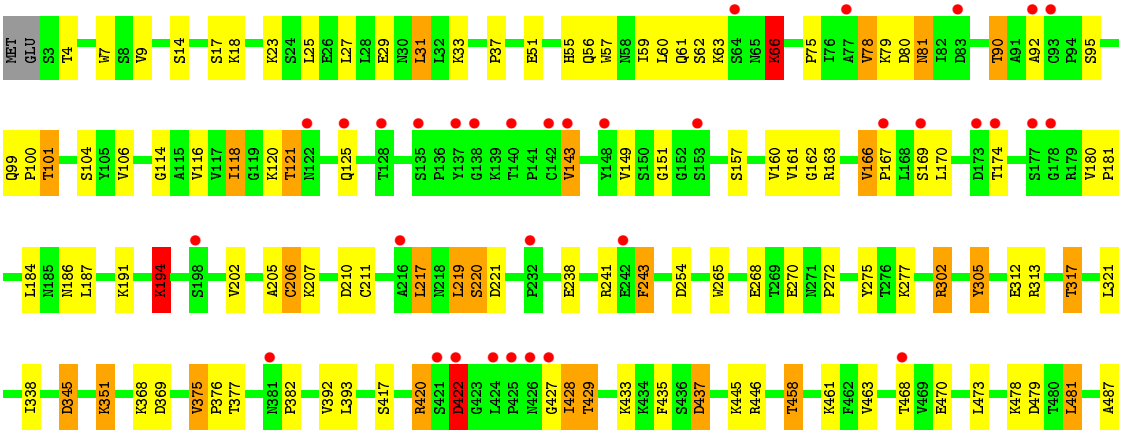
Chain C:

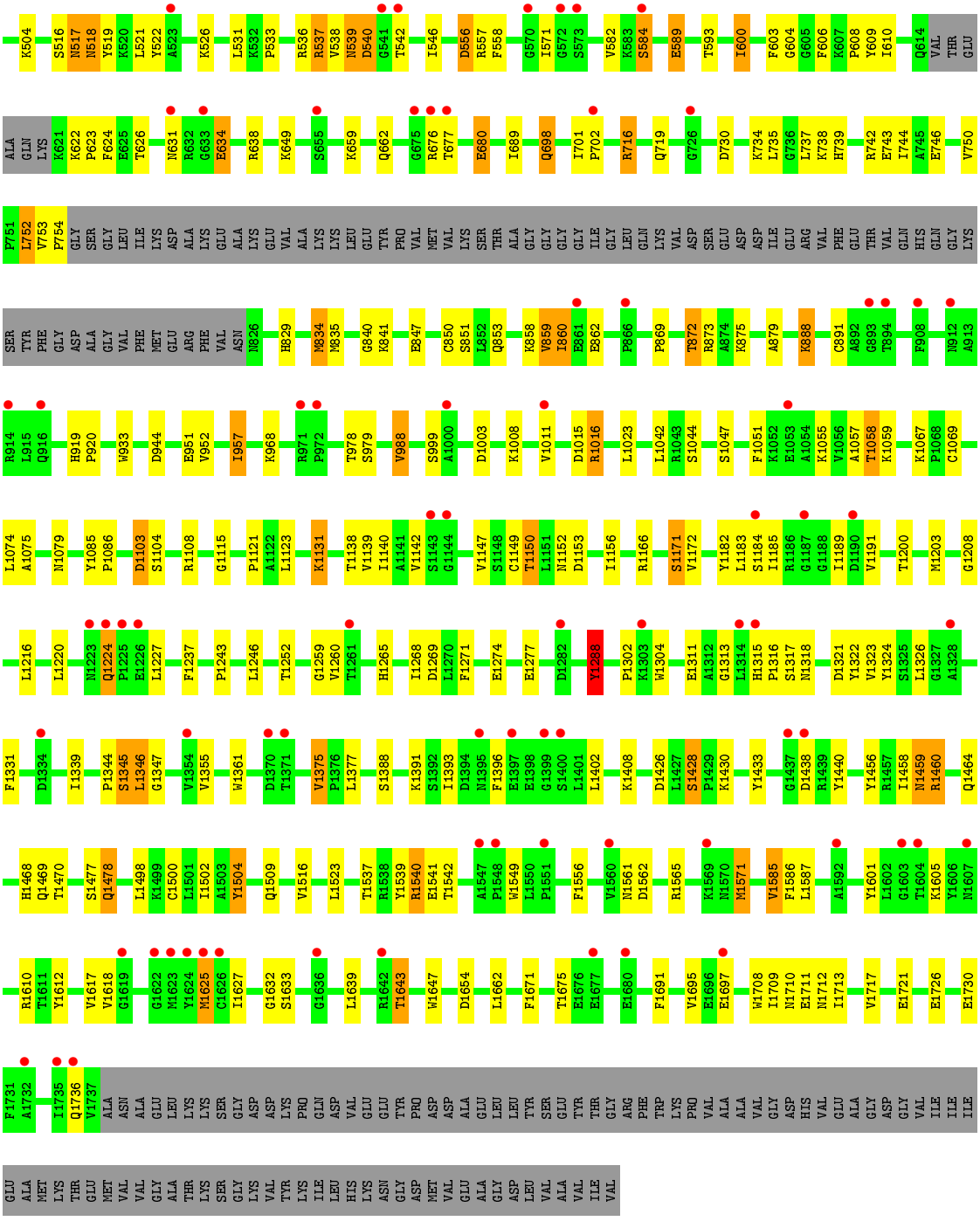




• Molecule 1: Urea Amidolyase

Chain D:




K504 S516 N517 N518 Y519 K520 L521 Y522 A523 K526 L531 K532 P533 R536 R537 V538 N539 D540 G541 T542 I546 D556 R557 F558 G570 I571 G572 S573 V582 K583 S584 E589 T593 I600 F603 G604 G605 F606 K607 P608 Y609 I610 Q614 VAL THR GLU
ALA GLN LYS K621 K622 P623 F624 E625 T626 N631 R632 G633 E634 R638 K649 S655 K659 Q662 G675 R676 T677 E680 I689 Q698 I701 P702 R716 Q719 G726 D730 K734 L735 G736 L737 K738 H739 R742 E743 I744 A745 E746 V750
P751 L752 V753 P754 GLY SER GLY LEU ILE LYS ASP ALA LYS GLU ALA LYS GLU VAL ALA LYS LYS LEU GLU TYR PRO VAL MET VAL LYS SER THR ALA GLY GLY GLY GLY ILE GLY LEU GLN LYS VAL ASP SER GLU ASP ASP ILE GLU ARG VAL PHE GLU THR VAL GLN HIS GLN GLY LYS
SER TYR PHE GLY ASP ALA GLY VAL PHE MET GLU ARG PHE VAL ASN N826 H829 M834 M835 G840 K841 E847 C850 S851 L852 Q853 K858 V859 I860 E861 E862 P866 P869 T872 R873 A874 K875 A879 K888 C891 A892 G893 T894 F908 N912 A913
R914 L915 Q916 H919 P920 W933 D944 E951 V952 I957 K968 R971 P972 T978 S979 V988 S999 A1000 D1003 K1008 V1011 D1015 R1016 L1023 L1042 R1043 S1044 S1047 F1051 K1052 E1053 A1054 K1055 V1056 A1057 T1058 K1059 K1067 P1068 C1069
L1074 A1075 N1079 Y1085 P1086 D1103 S1104 R1108 G1115 P1121 A1122 L1123 K1131 T1138 V1139 I1140 A1141 V1142 S1143 G1144 V1147 S1148 C1149 T1150 L1151 N1152 D1153 I1156 R1166 S1171 V1172 Y1182 L1183 S1184 I1185 R1186 G1187 G1188 I1189 D1190 V1191 T1200 M1203 G1208
L1216 L1220 N1223 Q1224 P1225 E1226 L1227 F1237 P1243 L1246 T1252 G1259 V1260 T1261 H1265 I1268 D1269 L1270 F1271 E1274 E1277 D1282 Y1288 P1302 K1303 W1304 E1311 A1312 G1313 L1314 H1315 P1316 S1317 N1318 D1321 Y1322 V1323 Y1324 S1325 L1326 G1327 A1328
F1331 D1334 I1339 P1344 S1345 L1346 G1347 V1354 V1355 W1361 D1370 T1371 V1375 P1376 L1377 S1388 K1391 S1392 I1393 D1394 N1395 F1396 E1397 E1398 G1399 S1400 L1401 L1402 K1408 D1426 L1427 S1428 P1429 K1430 Y1433 G1437 D1438 R1439 Y1440 Y1456 R1457 I1458 N1459 R1460 Q1464
H1468 Q1469 T1470 S1477 Q1478 L1498 K1499 C1500 L1501 I1502 A1503 Y1504 Q1509 V1516 L1523 T1537 R1538 Y1539 R1540 E1541 T1542 A1547 P1548 W1549 L1550 P1551 F1556 V1560 N1561 D1562 R1565 K1569 N1570 M1571 V1585 F1586 L1587 A1592 Y1601 L1602 G1603 T1604 K1605 Y1606 N1607
R1610 T1611 Y1612 V1617 V1618 G1619 G1622 M1623 Y1624 M1625 C1626 I1627 G1632 S1633 G1636 L1639 R1642 T1643 W1647 D1654 L1662 F1671 T1675 E1676 E1677 E1680 F1691 V1695 E1696 E1697 W1708 I1709 N1710 E1711 N1712 I1713 V1717 E1721 E1726 E1730
F1731 A1732 I1735 Q1736 V1737 ALA ASN ALA GLU LEU LYS LYS SER GLY ASP ASP LYS PRO GLN ASP VAL GLU GLU TYR PRO ASP ASP ALA GLU LEU LEU TYR SER GLU TYR THR GLY ARG PHE TRP LYS PRO VAL ALA ALA VAL GLY ASP HIS VAL GLU ALA GLY ASP GLY VAL ILE ILE ILE
GLU ALA MET LYS THR GLU MET VAL VAL GLY ALA THR LYS SER GLY LYS VAL TYR LYS ILE LEU HIS LYS ASN GLY ASP MET VAL GLU ALA GLY ASP LEU VAL ALA VAL ILE VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.74Å 181.94Å 549.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 6.50 29.98 – 6.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.98-6.50) 96.0 (29.98-6.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 6.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.278 , 0.302 0.279 , 0.305	Depositor DCC
R_{free} test set	1015 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	216.1	Xtriage
Anisotropy	0.897	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 249.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	51722	wwPDB-VP
Average B, all atoms (Å^2)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	1/13231 (0.0%)	0.70	4/17964 (0.0%)
1	B	0.51	2/13214 (0.0%)	0.86	23/17942 (0.1%)
1	C	0.39	1/13231 (0.0%)	0.69	5/17964 (0.0%)
1	D	0.49	3/13214 (0.0%)	0.83	21/17942 (0.1%)
All	All	0.45	7/52890 (0.0%)	0.77	53/71812 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	6
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1546	GLU	CG-CD	-7.32	1.41	1.51
1	C	1288	TYR	CD2-CE2	6.77	1.49	1.39
1	B	1546	GLU	CG-CD	-5.72	1.43	1.51
1	D	17	SER	CA-CB	5.61	1.61	1.52
1	D	1288	TYR	CD2-CE2	5.39	1.47	1.39
1	D	392	VAL	CB-CG1	5.13	1.63	1.52
1	B	392	VAL	CB-CG1	5.11	1.63	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	556	ASP	N-CA-CB	-8.99	94.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	556	ASP	N-CA-CB	-8.84	94.69	110.60
1	A	1504	TYR	CB-CG-CD1	-8.11	116.14	121.00
1	D	1504	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	D	422	ASP	N-CA-CB	-7.68	96.78	110.60
1	D	194	LYS	CD-CE-NZ	-7.39	94.70	111.70
1	D	254	ASP	CB-CA-C	-7.35	95.71	110.40
1	B	558	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	B	254	ASP	CB-CA-C	-7.26	95.88	110.40
1	B	66	LYS	CD-CE-NZ	7.15	128.15	111.70
1	D	118	ILE	CG1-CB-CG2	-6.92	96.17	111.40
1	D	558	PHE	CB-CG-CD1	-6.80	116.04	120.80
1	B	305	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	B	118	ILE	CG1-CB-CG2	-6.72	96.62	111.40
1	B	194	LYS	CD-CE-NZ	-6.68	96.34	111.70
1	B	1504	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	B	1303	LYS	N-CA-C	-6.47	93.52	111.00
1	D	1504	TYR	CB-CG-CD2	6.44	124.87	121.00
1	A	1504	TYR	CB-CG-CD2	6.36	124.81	121.00
1	D	305	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	457	ARG	CG-CD-NE	6.28	124.99	111.80
1	D	31	LEU	CA-CB-CG	6.10	129.32	115.30
1	B	305	TYR	CB-CG-CD1	6.04	124.62	121.00
1	D	305	TYR	CB-CG-CD1	5.97	124.58	121.00
1	B	217	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	217	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	1288	TYR	CA-CB-CG	-5.89	102.21	113.40
1	D	66	LYS	CD-CE-NZ	5.88	125.22	111.70
1	B	217	LEU	CB-CG-CD2	5.82	120.89	111.00
1	C	38	ALA	C-N-CD	5.82	140.61	128.40
1	D	531	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	C	1540	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	D	481	LEU	CA-CB-CG	5.77	128.58	115.30
1	B	519	TYR	N-CA-C	5.71	126.42	111.00
1	B	558	PHE	CB-CG-CD2	5.71	124.80	120.80
1	B	31	LEU	CA-CB-CG	5.69	128.39	115.30
1	D	217	LEU	CB-CG-CD2	5.68	120.66	111.00
1	A	38	ALA	C-N-CD	5.66	140.29	128.40
1	D	571	ILE	CG1-CB-CG2	-5.60	99.07	111.40
1	B	571	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	D	345	ASP	CB-CA-C	-5.56	99.28	110.40
1	B	481	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	64	SER	CB-CA-C	-5.38	99.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	558	PHE	CB-CG-CD2	5.37	124.56	120.80
1	B	345	ASP	CB-CA-C	-5.36	99.68	110.40
1	B	519	TYR	N-CA-CB	-5.28	101.10	110.60
1	B	464	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	D	1540	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	C	546	ILE	CG1-CB-CG2	-5.15	100.08	111.40
1	C	898	ILE	N-CA-C	-5.14	97.13	111.00
1	B	446	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	188	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	D	446	ARG	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1469	GLN	Mainchain
1	A	539	ASN	Peptide
1	B	1469	GLN	Mainchain
1	B	539	ASN	Peptide
1	C	1288	TYR	Mainchain
1	C	539	ASN	Peptide
1	C	896	GLU	Mainchain
1	D	101	THR	Mainchain
1	D	1288	TYR	Mainchain
1	D	382	PRO	Mainchain
1	D	422	ASP	Mainchain
1	D	517	ASN	Mainchain
1	D	539	ASN	Peptide

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	12939	0	12896	226	0
1	B	12922	0	12878	218	1
1	C	12939	0	12896	203	1
1	D	12922	0	12878	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	51722	0	51548	813	1

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 8.

All (813) 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:B:59:ILE:O	1:B:62:SER:OG	1.78	1.01
1:B:79:LYS:HA	1:B:121:THR:HG22	1.45	0.97
1:C:1509:GLN:NE2	1:D:101:THR:O	1.97	0.97
1:D:79:LYS:HA	1:D:121:THR:HG22	1.45	0.95
1:A:493:LEU:HB2	1:A:496:LEU:HD12	1.47	0.94
1:C:79:LYS:HA	1:C:121:THR:HG22	1.51	0.93
1:A:1546:GLU:HB2	1:D:1288:TYR:CD1	2.06	0.91
1:A:63:LYS:HA	1:B:1468:HIS:O	1.70	0.91
1:A:1288:TYR:OH	1:D:1541:GLU:HB3	1.72	0.89
1:A:1468:HIS:HE1	1:B:59:ILE:HG23	1.39	0.88
1:C:1459:ASN:HD21	1:C:1460:ARG:HH11	1.21	0.87
1:A:79:LYS:HA	1:A:121:THR:HG22	1.55	0.86
1:D:59:ILE:O	1:D:62:SER:OG	1.94	0.84
1:A:1459:ASN:HD21	1:A:1460:ARG:HH11	1.22	0.84
1:D:1459:ASN:HD21	1:D:1460:ARG:HH11	1.22	0.83
1:D:79:LYS:HG2	1:D:81:ASN:HB2	1.60	0.82
1:A:79:LYS:HG2	1:A:81:ASN:HB2	1.59	0.82
1:B:79:LYS:HG2	1:B:81:ASN:HB2	1.61	0.82
1:B:1459:ASN:HD21	1:B:1460:ARG:HH11	1.23	0.81
1:C:59:ILE:HG23	1:D:1468:HIS:HE1	1.43	0.80
1:C:79:LYS:HG2	1:C:81:ASN:HB2	1.64	0.80
1:A:1468:HIS:O	1:B:63:LYS:HA	1.82	0.80
1:A:58:ASN:O	1:A:62:SER:OG	2.01	0.79
1:D:859:VAL:HG23	1:D:860:ILE:HD12	1.63	0.79
1:D:186:ASN:HD21	1:D:458:THR:HG22	1.45	0.79
1:C:59:ILE:HG23	1:D:1468:HIS:CE1	2.17	0.78
1:A:859:VAL:HG23	1:A:860:ILE:HD12	1.65	0.77
1:B:1585:VAL:HG13	1:B:1586:PHE:CD1	2.21	0.76
1:D:1585:VAL:HG13	1:D:1586:PHE:CD1	2.21	0.76
1:A:64:SER:HA	1:B:1471:VAL:HG23	1.68	0.76
1:B:859:VAL:HG23	1:B:860:ILE:HD12	1.68	0.76
1:C:1585:VAL:HG13	1:C:1586:PHE:CD1	2.20	0.76
1:C:859:VAL:HG23	1:C:860:ILE:HD12	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1585:VAL:HG13	1:A:1586:PHE:CD1	2.21	0.75
1:A:1546:GLU:HB2	1:D:1288:TYR:HD1	1.49	0.75
1:B:1016:ARG:NH2	1:B:1051:PHE:O	2.19	0.75
1:A:1016:ARG:NH2	1:A:1051:PHE:O	2.21	0.73
1:C:62:SER:O	1:D:1470:THR:HA	1.89	0.73
1:C:1016:ARG:NH2	1:C:1051:PHE:O	2.22	0.73
1:B:186:ASN:HD21	1:B:458:THR:HG22	1.54	0.72
1:A:1625:MET:HE1	1:A:1627:ILE:HG13	1.71	0.72
1:C:1459:ASN:ND2	1:C:1460:ARG:HH11	1.87	0.72
1:C:493:LEU:HB2	1:C:496:LEU:HD12	1.70	0.72
1:D:1016:ARG:NH2	1:D:1051:PHE:O	2.23	0.72
1:A:1459:ASN:ND2	1:A:1460:ARG:HH11	1.87	0.71
1:B:275:TYR:HD1	1:B:428:ILE:HD11	1.55	0.71
1:C:1464:GLN:O	1:C:1468:HIS:HD2	1.73	0.71
1:D:1459:ASN:ND2	1:D:1460:ARG:HH11	1.88	0.71
1:A:1470:THR:HA	1:B:62:SER:O	1.91	0.71
1:A:1542:THR:O	1:D:1541:GLU:HG3	1.90	0.71
1:A:59:ILE:HG23	1:B:1468:HIS:HE1	1.56	0.71
1:B:1625:MET:HE1	1:B:1627:ILE:HG13	1.72	0.71
1:C:149:VAL:HG13	1:C:151:GLY:H	1.54	0.71
1:D:275:TYR:HD1	1:D:428:ILE:HD11	1.54	0.70
1:D:57:TRP:O	1:D:61:GLN:HG2	1.91	0.70
1:A:186:ASN:HD21	1:A:458:THR:HG22	1.57	0.70
1:A:1465:VAL:O	1:A:1469:GLN:N	2.25	0.69
1:B:1459:ASN:ND2	1:B:1460:ARG:HH11	1.90	0.69
1:C:186:ASN:HD21	1:C:458:THR:HG22	1.58	0.69
1:B:519:TYR:CE2	1:B:537:ARG:HB2	2.29	0.68
1:B:186:ASN:ND2	1:B:458:THR:HG22	2.08	0.67
1:D:1318:ASN:HD21	1:D:1605:LYS:H	1.43	0.67
1:C:1571:MET:HG2	1:C:1601:TYR:CE2	2.30	0.66
1:A:149:VAL:HG13	1:A:151:GLY:H	1.59	0.66
1:A:1287:HIS:CE1	1:A:1288:TYR:CE2	2.83	0.66
1:D:275:TYR:CD1	1:D:428:ILE:HD11	2.31	0.66
1:B:1313:GLY:HA3	1:B:1318:ASN:HD22	1.61	0.66
1:A:62:SER:O	1:B:1470:THR:HA	1.96	0.66
1:A:504:LYS:O	1:A:557:ARG:NH2	2.30	0.65
1:C:1625:MET:HE1	1:C:1627:ILE:HG13	1.77	0.65
1:B:90:THR:HG22	1:B:92:ALA:H	1.62	0.65
1:C:464:ASP:HA	1:C:466:ARG:HH21	1.62	0.65
1:D:186:ASN:ND2	1:D:458:THR:HG22	2.11	0.65
1:A:377:THR:HA	1:A:429:THR:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:TYR:CD1	1:B:428:ILE:HD11	2.32	0.65
1:C:63:LYS:HA	1:D:1468:HIS:O	1.97	0.64
1:C:377:THR:HA	1:C:429:THR:HG22	1.78	0.64
1:B:1318:ASN:HD21	1:B:1605:LYS:H	1.46	0.64
1:D:1428:SER:O	1:D:1428:SER:OG	2.13	0.64
1:C:1075:ALA:HB3	1:C:1131:LYS:HG2	1.80	0.64
1:C:504:LYS:O	1:C:557:ARG:NH2	2.30	0.64
1:A:464:ASP:HA	1:A:466:ARG:HH21	1.62	0.64
1:C:62:SER:HB3	1:D:1504:TYR:OH	1.99	0.63
1:B:626:THR:HG22	1:B:649:LYS:HB2	1.79	0.63
1:A:1468:HIS:ND1	1:B:62:SER:OG	2.31	0.63
1:D:1464:GLN:O	1:D:1468:HIS:HD2	1.81	0.63
1:D:121:THR:HG21	1:D:157:SER:OG	1.99	0.63
1:D:1625:MET:HE1	1:D:1627:ILE:HG13	1.79	0.63
1:B:1150:THR:HG23	1:B:1153:ASP:H	1.64	0.63
1:B:205:ALA:O	1:B:206:CYS:HB2	1.99	0.63
1:A:1288:TYR:OH	1:D:1541:GLU:OE2	2.10	0.63
1:B:1466:GLU:C	1:B:1469:GLN:H	2.03	0.63
1:B:220:SER:HB2	1:B:470:GLU:O	1.99	0.63
1:A:1428:SER:O	1:A:1428:SER:OG	2.17	0.62
1:D:205:ALA:O	1:D:206:CYS:HB2	1.99	0.62
1:C:1470:THR:HA	1:D:62:SER:O	1.99	0.62
1:B:121:THR:HG21	1:B:157:SER:OG	1.99	0.62
1:C:1537:THR:O	1:C:1541:GLU:HG2	2.00	0.62
1:A:163:ARG:HG3	1:A:165:ILE:HD13	1.82	0.62
1:C:1150:THR:HG23	1:C:1153:ASP:H	1.64	0.62
1:A:477:SER:OG	1:A:479:ASP:HB2	2.00	0.61
1:A:64:SER:N	1:B:1469:GLN:O	2.33	0.61
1:B:1075:ALA:HB3	1:B:1131:LYS:HG2	1.80	0.61
1:D:90:THR:HG22	1:D:92:ALA:H	1.64	0.61
1:A:1075:ALA:HB3	1:A:1131:LYS:HG2	1.82	0.61
1:C:162:GLY:HA2	1:C:187:LEU:HD21	1.83	0.61
1:D:1150:THR:HG23	1:D:1153:ASP:H	1.65	0.61
1:D:220:SER:HB2	1:D:470:GLU:O	2.00	0.61
1:A:205:ALA:O	1:A:206:CYS:HB2	2.00	0.61
1:B:1708:TRP:HE3	1:B:1709:ILE:HD12	1.63	0.61
1:C:101:THR:O	1:D:1509:GLN:NE2	2.33	0.61
1:C:205:ALA:O	1:C:206:CYS:HB2	2.00	0.61
1:D:1571:MET:HG2	1:D:1601:TYR:CE2	2.34	0.61
1:A:742:ARG:HH22	1:A:753:VAL:HB	1.66	0.61
1:B:1339:ILE:HG23	1:B:1344:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1287:HIS:CE1	1:B:1288:TYR:CE2	2.89	0.61
1:A:90:THR:HG22	1:A:92:ALA:H	1.64	0.61
1:D:1075:ALA:HB3	1:D:1131:LYS:HG2	1.82	0.61
1:B:377:THR:HA	1:B:429:THR:HG22	1.83	0.61
1:B:57:TRP:O	1:B:61:GLN:HG2	2.01	0.60
1:A:1150:THR:HG23	1:A:1153:ASP:H	1.66	0.60
1:A:59:ILE:HG23	1:B:1468:HIS:CE1	2.37	0.60
1:D:1260:VAL:HG12	1:D:1355:VAL:HA	1.84	0.60
1:D:149:VAL:HG13	1:D:151:GLY:H	1.67	0.60
1:B:149:VAL:HG13	1:B:151:GLY:H	1.66	0.60
1:D:600:ILE:HD11	1:D:609:TYR:CE1	2.36	0.60
1:C:1339:ILE:HG23	1:C:1344:PRO:HD2	1.83	0.60
1:C:90:THR:HG22	1:C:92:ALA:H	1.66	0.60
1:D:1313:GLY:HA3	1:D:1318:ASN:HD22	1.67	0.60
1:B:1465:VAL:O	1:B:1469:GLN:N	2.35	0.60
1:A:1259:GLY:HA2	1:A:1375:VAL:HG12	1.84	0.59
1:B:1500:CYS:HB3	1:B:1504:TYR:CZ	2.36	0.59
1:D:1339:ILE:HG23	1:D:1344:PRO:HD2	1.83	0.59
1:D:60:LEU:HD11	1:D:114:GLY:HA2	1.83	0.59
1:C:1468:HIS:HE1	1:D:59:ILE:HG12	1.66	0.59
1:A:162:GLY:HA2	1:A:187:LEU:HD21	1.85	0.59
1:B:375:VAL:HG12	1:B:429:THR:HG23	1.84	0.59
1:B:478:LYS:O	1:B:481:LEU:HG	2.02	0.59
1:C:1428:SER:O	1:C:1428:SER:OG	2.18	0.59
1:D:375:VAL:HG12	1:D:429:THR:HG23	1.85	0.59
1:B:143:VAL:HG13	1:B:461:LYS:HB3	1.84	0.59
1:D:1708:TRP:HE3	1:D:1709:ILE:HD12	1.67	0.59
1:C:163:ARG:HG3	1:C:165:ILE:HD13	1.84	0.59
1:D:626:THR:HG22	1:D:649:LYS:HB2	1.85	0.59
1:D:377:THR:HA	1:D:429:THR:HG22	1.84	0.59
1:A:1708:TRP:HE3	1:A:1709:ILE:HD12	1.68	0.59
1:B:1260:VAL:HG12	1:B:1355:VAL:HA	1.83	0.59
1:D:519:TYR:CE2	1:D:537:ARG:HB2	2.37	0.59
1:A:186:ASN:ND2	1:A:458:THR:HG22	2.16	0.59
1:B:1428:SER:OG	1:B:1428:SER:O	2.18	0.59
1:C:1708:TRP:HE3	1:C:1709:ILE:HD12	1.66	0.59
1:C:626:THR:HG22	1:C:649:LYS:HB2	1.85	0.59
1:A:1469:GLN:HB3	1:B:64:SER:OG	2.02	0.58
1:B:1121:PRO:HG2	1:B:1189:ILE:H	1.68	0.58
1:C:186:ASN:ND2	1:C:458:THR:HG22	2.18	0.58
1:C:477:SER:OG	1:C:479:ASP:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1121:PRO:HG2	1:D:1189:ILE:H	1.66	0.58
1:A:603:PHE:HB3	1:A:608:PRO:HB2	1.84	0.58
1:C:742:ARG:HH22	1:C:753:VAL:HB	1.69	0.58
1:D:1131:LYS:HB3	1:D:1171:SER:HB2	1.84	0.58
1:A:320:PHE:O	1:A:323:THR:HB	2.03	0.58
1:A:600:ILE:HD11	1:A:609:TYR:CZ	2.38	0.58
1:B:600:ILE:HD11	1:B:609:TYR:CE1	2.39	0.58
1:D:478:LYS:O	1:D:481:LEU:HG	2.03	0.58
1:A:1571:MET:HG2	1:A:1601:TYR:CE2	2.37	0.58
1:B:317:THR:HG21	1:B:338:ILE:HG21	1.84	0.58
1:A:1260:VAL:HG12	1:A:1355:VAL:HA	1.85	0.58
1:D:317:THR:HG21	1:D:338:ILE:HG21	1.85	0.58
1:B:1131:LYS:HB3	1:B:1171:SER:HB2	1.85	0.58
1:C:56:GLN:O	1:C:59:ILE:HB	2.03	0.58
1:B:742:ARG:HH22	1:B:753:VAL:HB	1.67	0.58
1:C:1131:LYS:HB3	1:C:1171:SER:HB2	1.86	0.58
1:A:1339:ILE:HG23	1:A:1344:PRO:HD2	1.84	0.58
1:B:1259:GLY:HA2	1:B:1375:VAL:HG12	1.86	0.58
1:A:1131:LYS:HB3	1:A:1171:SER:HB2	1.86	0.57
1:C:1464:GLN:O	1:C:1468:HIS:CD2	2.55	0.57
1:C:375:VAL:HG12	1:C:429:THR:HG23	1.85	0.57
1:D:853:GLN:HG2	1:D:858:LYS:HG2	1.86	0.57
1:C:600:ILE:HD11	1:C:609:TYR:CZ	2.39	0.57
1:D:1587:LEU:HB3	1:D:1647:TRP:CD2	2.39	0.57
1:A:1713:ILE:O	1:A:1717:VAL:HG23	2.05	0.57
1:C:603:PHE:HB3	1:C:608:PRO:HB2	1.86	0.57
1:D:1085:TYR:CD2	1:D:1108:ARG:HD3	2.39	0.57
1:A:1121:PRO:HG2	1:A:1189:ILE:H	1.70	0.57
1:B:603:PHE:HB3	1:B:608:PRO:HB2	1.86	0.57
1:C:1069:CYS:SG	1:C:1224:GLN:HB2	2.45	0.57
1:A:1466:GLU:C	1:A:1469:GLN:H	2.07	0.56
1:B:1587:LEU:HB3	1:B:1647:TRP:CD2	2.40	0.56
1:D:742:ARG:HH22	1:D:753:VAL:HB	1.70	0.56
1:C:1085:TYR:CD2	1:C:1108:ARG:HD3	2.40	0.56
1:D:1315:HIS:HD2	1:D:1317:SER:H	1.52	0.56
1:D:752:LEU:HD12	1:D:752:LEU:H	1.70	0.56
1:C:1121:PRO:HG2	1:C:1189:ILE:H	1.71	0.56
1:A:752:LEU:HD12	1:A:752:LEU:H	1.71	0.56
1:B:1069:CYS:SG	1:B:1224:GLN:HB2	2.46	0.56
1:B:417:SER:OG	1:B:427:GLY:HA2	2.04	0.56
1:A:1085:TYR:CD2	1:A:1108:ARG:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:O	1:A:66:LYS:NZ	2.29	0.56
1:B:504:LYS:O	1:B:557:ARG:NH2	2.39	0.56
1:C:853:GLN:HG2	1:C:858:LYS:HG2	1.86	0.56
1:C:957:ILE:HG12	1:C:1023:LEU:HD22	1.86	0.56
1:A:1458:ILE:HG21	1:A:1478:GLN:HG2	1.88	0.56
1:D:265:TRP:CD2	1:D:272:PRO:HG3	2.41	0.56
1:C:320:PHE:O	1:C:323:THR:HB	2.06	0.56
1:B:853:GLN:HG2	1:B:858:LYS:HG2	1.88	0.56
1:C:1587:LEU:HB3	1:C:1647:TRP:CD2	2.40	0.55
1:D:417:SER:OG	1:D:427:GLY:HA2	2.06	0.55
1:C:1468:HIS:CE1	1:D:59:ILE:HG23	2.40	0.55
1:A:1587:LEU:HB3	1:A:1647:TRP:CD2	2.42	0.55
1:D:1713:ILE:O	1:D:1717:VAL:HG23	2.06	0.55
1:B:61:GLN:O	1:B:66:LYS:NZ	2.32	0.55
1:A:853:GLN:HG2	1:A:858:LYS:HG2	1.88	0.55
1:D:174:THR:OG1	1:D:210:ASP:OD1	2.24	0.55
1:C:57:TRP:O	1:C:61:GLN:HG2	2.06	0.55
1:A:626:THR:HG22	1:A:649:LYS:HB2	1.88	0.55
1:B:1464:GLN:O	1:B:1468:HIS:HD2	1.88	0.55
1:A:121:THR:HG21	1:A:157:SER:OG	2.06	0.55
1:A:1500:CYS:HB3	1:A:1504:TYR:CZ	2.42	0.55
1:A:375:VAL:HG12	1:A:429:THR:HG23	1.89	0.55
1:C:1571:MET:HG2	1:C:1601:TYR:HE2	1.70	0.55
1:B:80:ASP:OD1	1:B:90:THR:HB	2.07	0.55
1:C:1713:ILE:O	1:C:1717:VAL:HG23	2.06	0.55
1:B:1085:TYR:CD2	1:B:1108:ARG:HD3	2.42	0.54
1:B:1189:ILE:HG21	1:B:1220:LEU:HD23	1.89	0.54
1:A:57:TRP:O	1:A:61:GLN:HG2	2.07	0.54
1:B:1458:ILE:HG21	1:B:1478:GLN:HG2	1.89	0.54
1:C:1260:VAL:HG12	1:C:1355:VAL:HA	1.88	0.54
1:B:957:ILE:HG12	1:B:1023:LEU:HD22	1.89	0.54
1:D:504:LYS:O	1:D:557:ARG:NH2	2.39	0.54
1:A:1561:ASN:ND2	1:A:1601:TYR:HB3	2.21	0.54
1:D:80:ASP:OD1	1:D:90:THR:HB	2.07	0.54
1:A:65:ASN:O	1:A:68:GLU:HB2	2.07	0.54
1:B:847:GLU:OE2	1:B:873:ARG:NH1	2.41	0.54
1:C:1458:ILE:HG21	1:C:1478:GLN:HG2	1.90	0.54
1:A:295:GLU:HB3	1:A:296:PRO:HD3	1.90	0.54
1:A:607:LYS:HB2	1:A:608:PRO:CD	2.38	0.54
1:C:607:LYS:HB2	1:C:608:PRO:CD	2.38	0.54
1:A:1069:CYS:SG	1:A:1224:GLN:HB2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:VAL:HB	1:D:221:ASP:OD1	2.07	0.54
1:B:1561:ASN:ND2	1:B:1601:TYR:HB3	2.22	0.54
1:D:603:PHE:HB3	1:D:608:PRO:HB2	1.89	0.54
1:A:80:ASP:OD1	1:A:90:THR:HB	2.08	0.54
1:A:1200:THR:OG1	1:A:1208:GLY:HA3	2.09	0.53
1:A:847:GLU:OE2	1:A:873:ARG:NH1	2.42	0.53
1:A:1543:ILE:O	1:D:1542:THR:HA	2.08	0.53
1:B:487:ALA:HB3	1:B:584:SER:HB2	1.91	0.53
1:C:1710:ASN:C	1:C:1712:ASN:H	2.12	0.53
1:C:295:GLU:HB3	1:C:296:PRO:HD3	1.89	0.53
1:A:634:GLU:OE1	1:A:1008:LYS:HE2	2.09	0.53
1:D:1189:ILE:HG21	1:D:1220:LEU:HD23	1.90	0.53
1:A:624:PHE:HD1	1:A:698:GLN:HG3	1.74	0.53
1:A:62:SER:HB3	1:B:1504:TYR:CE2	2.44	0.53
1:C:592:TYR:OH	1:D:589:GLU:HG3	2.09	0.53
1:B:265:TRP:CD2	1:B:272:PRO:HG3	2.44	0.53
1:C:634:GLU:OE1	1:C:1008:LYS:HE2	2.09	0.53
1:D:957:ILE:HG12	1:D:1023:LEU:HD22	1.90	0.53
1:A:957:ILE:HG12	1:A:1023:LEU:HD22	1.90	0.53
1:B:1459:ASN:ND2	1:B:1460:ARG:HD2	2.24	0.53
1:D:1259:GLY:HA2	1:D:1375:VAL:HG12	1.91	0.53
1:C:1503:ALA:HB1	1:D:55:HIS:CD2	2.44	0.53
1:A:1149:CYS:HB2	1:A:1156:ILE:HG22	1.91	0.52
1:A:1459:ASN:ND2	1:A:1460:ARG:HD2	2.24	0.52
1:C:80:ASP:OD1	1:C:90:THR:HB	2.09	0.52
1:D:375:VAL:HG13	1:D:376:PRO:O	2.09	0.52
1:A:92:ALA:HB3	1:A:125:GLN:HA	1.90	0.52
1:A:163:ARG:HG3	1:A:165:ILE:CD1	2.39	0.52
1:A:607:LYS:HB2	1:A:608:PRO:HD3	1.91	0.52
1:D:56:GLN:O	1:D:59:ILE:HB	2.10	0.52
1:A:125:GLN:HG2	1:A:126:PHE:CD1	2.45	0.52
1:B:174:THR:OG1	1:B:210:ASP:OD1	2.27	0.52
1:C:600:ILE:HD11	1:C:609:TYR:CE1	2.45	0.52
1:C:375:VAL:CG1	1:C:401:TRP:HB3	2.40	0.52
1:D:634:GLU:OE1	1:D:1008:LYS:HE2	2.09	0.52
1:D:1459:ASN:ND2	1:D:1460:ARG:HD2	2.24	0.52
1:A:1189:ILE:HG21	1:A:1220:LEU:HD23	1.91	0.52
1:C:1459:ASN:ND2	1:C:1460:ARG:HD2	2.25	0.52
1:A:1710:ASN:C	1:A:1712:ASN:H	2.13	0.52
1:B:375:VAL:HG13	1:B:376:PRO:O	2.10	0.52
1:D:1571:MET:HG2	1:D:1601:TYR:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:HIS:HE1	1:A:1322:TYR:CZ	2.28	0.52
1:A:592:TYR:OH	1:B:589:GLU:HG3	2.10	0.52
1:B:143:VAL:HG22	1:B:163:ARG:HG3	1.91	0.52
1:B:919:HIS:ND1	1:B:920:PRO:HD3	2.25	0.52
1:C:835:MET:HG2	1:C:933:TRP:HE3	1.75	0.52
1:C:829:HIS:CD2	1:C:850:CYS:HB2	2.45	0.52
1:D:1200:THR:OG1	1:D:1208:GLY:HA3	2.09	0.52
1:D:1458:ILE:HG21	1:D:1478:GLN:HG2	1.91	0.52
1:A:835:MET:HG2	1:A:933:TRP:HE3	1.74	0.52
1:A:1288:TYR:CZ	1:D:1541:GLU:HB3	2.45	0.52
1:A:589:GLU:O	1:A:593:THR:HB	2.09	0.51
1:A:75:PRO:O	1:A:166:VAL:HG22	2.11	0.51
1:B:60:LEU:HD11	1:B:114:GLY:HA2	1.91	0.51
1:B:9:VAL:HB	1:B:221:ASP:OD1	2.11	0.51
1:C:1189:ILE:HG21	1:C:1220:LEU:HD23	1.91	0.51
1:C:65:ASN:O	1:C:68:GLU:HB2	2.10	0.51
1:C:1259:GLY:HA2	1:C:1375:VAL:HG12	1.91	0.51
1:C:752:LEU:H	1:C:752:LEU:HD12	1.75	0.51
1:C:1469:GLN:HB2	1:D:63:LYS:HA	1.93	0.51
1:A:1288:TYR:CD1	1:A:1288:TYR:C	2.83	0.51
1:A:600:ILE:HD11	1:A:609:TYR:CE1	2.46	0.51
1:C:607:LYS:HB2	1:C:608:PRO:HD3	1.91	0.51
1:D:1498:LEU:O	1:D:1502:ILE:HG12	2.11	0.51
1:A:59:ILE:HD13	1:A:111:ARG:NH2	2.26	0.51
1:B:1315:HIS:HD2	1:B:1317:SER:H	1.58	0.51
1:B:1498:LEU:O	1:B:1502:ILE:HG12	2.11	0.51
1:C:92:ALA:HB3	1:C:125:GLN:HA	1.91	0.51
1:C:589:GLU:O	1:C:593:THR:HB	2.11	0.51
1:C:847:GLU:OE2	1:C:873:ARG:NH1	2.44	0.51
1:C:869:PRO:HD2	1:C:872:THR:CG2	2.41	0.51
1:D:487:ALA:HB3	1:D:584:SER:HB2	1.93	0.51
1:D:869:PRO:HD2	1:D:872:THR:CG2	2.41	0.51
1:B:351:LYS:O	1:B:351:LYS:HE3	2.11	0.51
1:D:1710:ASN:C	1:D:1712:ASN:H	2.13	0.51
1:A:63:LYS:O	1:A:66:LYS:NZ	2.34	0.51
1:B:1265:HIS:HE1	1:B:1322:TYR:CZ	2.28	0.51
1:D:829:HIS:CD2	1:D:850:CYS:HB2	2.47	0.50
1:C:125:GLN:HG2	1:C:126:PHE:CD1	2.47	0.50
1:C:62:SER:HB2	1:D:1468:HIS:HB3	1.93	0.50
1:D:1625:MET:HE3	1:D:1671:PHE:HZ	1.76	0.50
1:A:1470:THR:HB	1:A:1473:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1345:SER:OG	1:B:1346:LEU:N	2.44	0.50
1:B:1545:SER:C	1:B:1546:GLU:HG3	2.31	0.50
1:C:1149:CYS:HB2	1:C:1156:ILE:HG22	1.93	0.50
1:C:290:VAL:HG12	1:C:292:VAL:HG23	1.92	0.50
1:D:677:THR:OG1	1:D:680:GLU:HB2	2.12	0.50
1:A:1466:GLU:O	1:A:1469:GLN:HG3	2.12	0.50
1:D:143:VAL:HG13	1:D:461:LYS:HB3	1.94	0.50
1:A:1288:TYR:OH	1:D:1541:GLU:CB	2.54	0.50
1:B:1149:CYS:HB2	1:B:1156:ILE:HG22	1.93	0.50
1:B:610:ILE:O	1:B:610:ILE:HG22	2.12	0.50
1:C:1200:THR:OG1	1:C:1208:GLY:HA3	2.11	0.50
1:D:1140:ILE:HD11	1:D:1185:ILE:HD12	1.94	0.50
1:A:750:VAL:HG22	1:A:879:ALA:HB1	1.94	0.50
1:A:62:SER:HB2	1:B:1468:HIS:ND1	2.27	0.50
1:B:1625:MET:HE3	1:B:1671:PHE:HZ	1.77	0.50
1:D:219:LEU:HB3	1:D:473:LEU:HD21	1.94	0.50
1:A:1203:MET:HE1	1:A:1633:SER:HB3	1.94	0.49
1:B:634:GLU:OE1	1:B:1008:LYS:HE2	2.13	0.49
1:B:317:THR:HG23	1:B:321:LEU:HD12	1.94	0.49
1:A:1287:HIS:CE1	1:A:1288:TYR:CZ	3.00	0.49
1:A:194:LYS:HG2	1:A:211:CYS:SG	2.52	0.49
1:B:1625:MET:CE	1:B:1627:ILE:HG13	2.41	0.49
1:C:420:ARG:HG3	1:C:424:LEU:O	2.11	0.49
1:D:1324:TYR:CZ	1:D:1347:GLY:HA3	2.47	0.49
1:A:1498:LEU:O	1:A:1502:ILE:HG12	2.13	0.49
1:A:417:SER:OG	1:A:427:GLY:HA2	2.12	0.49
1:A:487:ALA:HB3	1:A:584:SER:HB2	1.93	0.49
1:B:1464:GLN:O	1:B:1468:HIS:CD2	2.65	0.49
1:C:1345:SER:OG	1:C:1346:LEU:N	2.45	0.49
1:A:611:GLU:C	1:A:613:ILE:H	2.15	0.49
1:C:1115:GLY:HA2	1:C:1237:PHE:HB2	1.93	0.49
1:C:163:ARG:HG3	1:C:165:ILE:CD1	2.41	0.49
1:D:835:MET:HG2	1:D:933:TRP:HE3	1.77	0.49
1:A:1203:MET:CE	1:A:1633:SER:HB3	2.42	0.49
1:C:1498:LEU:O	1:C:1502:ILE:HG12	2.13	0.49
1:D:1537:THR:O	1:D:1541:GLU:HG2	2.12	0.49
1:D:1625:MET:CE	1:D:1627:ILE:HG13	2.43	0.49
1:D:847:GLU:OE2	1:D:873:ARG:NH1	2.46	0.49
1:A:1464:GLN:O	1:A:1468:HIS:HD2	1.95	0.49
1:A:375:VAL:CG1	1:A:401:TRP:HB3	2.42	0.49
1:D:1269:ASP:OD2	1:D:1269:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1500:CYS:HB3	1:D:1504:TYR:CZ	2.48	0.49
1:A:1184:SER:C	1:A:1185:ILE:HD13	2.33	0.49
1:B:1200:THR:OG1	1:B:1208:GLY:HA3	2.13	0.49
1:A:1345:SER:OG	1:A:1346:LEU:N	2.46	0.49
1:B:162:GLY:HA2	1:B:187:LEU:HD21	1.95	0.49
1:B:452:PHE:CD1	1:B:457:ARG:HG3	2.48	0.49
1:B:677:THR:OG1	1:B:680:GLU:HB2	2.13	0.49
1:B:869:PRO:HD2	1:B:872:THR:CG2	2.43	0.49
1:D:1274:GLU:HA	1:D:1277:GLU:HG3	1.95	0.49
1:C:1468:HIS:CE1	1:D:59:ILE:HG12	2.48	0.49
1:A:1625:MET:CE	1:A:1627:ILE:HG13	2.42	0.49
1:D:1265:HIS:HE1	1:D:1322:TYR:CZ	2.31	0.49
1:D:317:THR:HG23	1:D:321:LEU:HD12	1.95	0.49
1:A:1617:VAL:HG11	1:A:1639:LEU:HD22	1.95	0.48
1:A:66:LYS:O	1:A:67:GLU:HB2	2.13	0.48
1:B:180:VAL:HB	1:B:181:PRO:HD3	1.95	0.48
1:A:75:PRO:HB2	1:A:118:ILE:CD1	2.43	0.48
1:B:1470:THR:HB	1:B:1473:ILE:HD12	1.96	0.48
1:B:1571:MET:HG2	1:B:1601:TYR:CE2	2.48	0.48
1:C:121:THR:HG21	1:C:157:SER:OG	2.12	0.48
1:C:1553:ASN:OD1	1:C:1606:TYR:OH	2.24	0.48
1:A:1537:THR:O	1:A:1541:GLU:HG2	2.14	0.48
1:A:536:ARG:HD3	1:A:538:VAL:HG23	1.95	0.48
1:B:420:ARG:HB2	1:B:422:ASP:HB2	1.95	0.48
1:D:539:ASN:O	1:D:540:ASP:O	2.31	0.48
1:A:290:VAL:HG12	1:A:292:VAL:HG23	1.95	0.48
1:B:1103:ASP:OD2	1:B:1361:TRP:HB2	2.14	0.48
1:C:536:ARG:HD3	1:C:538:VAL:HG23	1.94	0.48
1:D:92:ALA:HB3	1:D:125:GLN:HA	1.94	0.48
1:D:243:PHE:CZ	1:D:435:PHE:HA	2.49	0.48
1:C:1468:HIS:O	1:D:63:LYS:HA	2.13	0.48
1:A:1467:ARG:NH2	1:B:112:ASP:OD2	2.47	0.48
1:C:1104:SER:O	1:C:1108:ARG:HG3	2.13	0.48
1:C:16:HIS:ND1	1:C:24:SER:HB2	2.28	0.48
1:D:1069:CYS:SG	1:D:1224:GLN:HB2	2.53	0.48
1:B:99:GLN:NE2	1:B:100:PRO:HD2	2.28	0.48
1:C:1265:HIS:HE1	1:C:1322:TYR:CZ	2.31	0.48
1:D:1345:SER:OG	1:D:1346:LEU:N	2.47	0.48
1:D:7:TRP:O	1:D:167:PRO:HB3	2.14	0.48
1:A:1324:TYR:CZ	1:A:1347:GLY:HA3	2.49	0.48
1:A:919:HIS:ND1	1:A:920:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:SER:C	1:B:1185:ILE:HD13	2.34	0.48
1:C:624:PHE:HD1	1:C:698:GLN:HG3	1.79	0.48
1:D:610:ILE:HG22	1:D:610:ILE:O	2.14	0.48
1:A:1115:GLY:HA2	1:A:1237:PHE:HB2	1.94	0.48
1:D:162:GLY:HA2	1:D:187:LEU:HD21	1.96	0.48
1:A:1587:LEU:HD12	1:A:1630:ALA:HB2	1.96	0.48
1:B:219:LEU:HB3	1:B:473:LEU:HD21	1.95	0.48
1:B:539:ASN:O	1:B:540:ASP:O	2.32	0.48
1:D:1149:CYS:HB2	1:D:1156:ILE:HG22	1.96	0.48
1:D:1561:ASN:ND2	1:D:1601:TYR:HB3	2.28	0.48
1:A:1269:ASP:OD2	1:A:1269:ASP:N	2.46	0.47
1:A:634:GLU:CD	1:A:1008:LYS:HE2	2.35	0.47
1:C:1184:SER:C	1:C:1185:ILE:HD13	2.34	0.47
1:C:377:THR:HA	1:C:429:THR:CG2	2.44	0.47
1:A:1545:SER:C	1:A:1546:GLU:HG3	2.34	0.47
1:C:1324:TYR:CZ	1:C:1347:GLY:HA3	2.49	0.47
1:A:1542:THR:HB	1:D:1541:GLU:OE1	2.14	0.47
1:A:420:ARG:HG3	1:A:424:LEU:O	2.13	0.47
1:A:492:HIS:NE2	1:A:501:GLN:OE1	2.41	0.47
1:B:1585:VAL:HG13	1:B:1586:PHE:HD1	1.75	0.47
1:D:1459:ASN:HD22	1:D:1460:ARG:HD2	1.80	0.47
1:D:919:HIS:ND1	1:D:920:PRO:HD3	2.29	0.47
1:C:677:THR:OG1	1:C:680:GLU:HB2	2.14	0.47
1:C:85:LYS:HD3	1:D:1509:GLN:NE2	2.28	0.47
1:D:351:LYS:O	1:D:351:LYS:HE3	2.14	0.47
1:A:1142:VAL:HA	1:A:1182:TYR:O	2.15	0.47
1:C:1587:LEU:HD12	1:C:1630:ALA:HB2	1.96	0.47
1:C:1625:MET:CE	1:C:1627:ILE:HG13	2.44	0.47
1:C:1708:TRP:CE3	1:C:1709:ILE:HD12	2.49	0.47
1:C:492:HIS:NE2	1:C:501:GLN:OE1	2.45	0.47
1:D:1103:ASP:OD2	1:D:1361:TRP:HB2	2.14	0.47
1:D:1464:GLN:O	1:D:1468:HIS:CD2	2.64	0.47
1:A:1059:LYS:HA	1:A:1059:LYS:HD2	1.75	0.47
1:B:1708:TRP:CE3	1:B:1709:ILE:HD12	2.48	0.47
1:B:546:ILE:N	1:B:546:ILE:HD12	2.30	0.47
1:C:919:HIS:ND1	1:C:920:PRO:HD3	2.29	0.47
1:D:78:VAL:HG22	1:D:120:LYS:HE3	1.96	0.47
1:D:1115:GLY:HA2	1:D:1237:PHE:HB2	1.96	0.47
1:A:862:GLU:OE1	1:A:1016:ARG:NH1	2.47	0.47
1:B:1587:LEU:HD12	1:B:1630:ALA:HB2	1.97	0.47
1:C:634:GLU:CD	1:C:1008:LYS:HE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLN:NE2	1:D:100:PRO:HD2	2.29	0.47
1:D:1184:SER:C	1:D:1185:ILE:HD13	2.35	0.47
1:C:1585:VAL:HG13	1:C:1586:PHE:HD1	1.75	0.47
1:B:1259:GLY:HA3	1:B:1377:LEU:HD22	1.97	0.47
1:C:1561:ASN:ND2	1:C:1601:TYR:HB3	2.30	0.47
1:C:417:SER:OG	1:C:427:GLY:HA2	2.15	0.47
1:D:546:ILE:HD12	1:D:546:ILE:N	2.29	0.47
1:D:622:LYS:HE3	1:D:622:LYS:HB2	1.67	0.47
1:A:1459:ASN:HD22	1:A:1460:ARG:HD2	1.80	0.47
1:B:1269:ASP:OD2	1:B:1269:ASP:N	2.47	0.47
1:B:302:ARG:HE	1:B:302:ARG:HB3	1.47	0.47
1:A:1140:ILE:HD11	1:A:1185:ILE:HD12	1.96	0.46
1:A:78:VAL:HG22	1:A:120:LYS:HE3	1.96	0.46
1:A:1288:TYR:CD1	1:A:1289:ASN:N	2.84	0.46
1:A:521:LEU:HB2	1:A:546:ILE:HG12	1.97	0.46
1:B:1275:TYR:HB2	1:B:1303:LYS:HG3	1.98	0.46
1:B:1713:ILE:O	1:B:1717:VAL:HG23	2.15	0.46
1:B:14:SER:O	1:B:18:LYS:HG2	2.15	0.46
1:C:1:MET:HB2	1:C:2:GLU:H	1.60	0.46
1:C:61:GLN:O	1:C:66:LYS:NZ	2.40	0.46
1:A:377:THR:HA	1:A:429:THR:CG2	2.43	0.46
1:A:38:ALA:HB1	1:A:39:PRO:HD3	1.97	0.46
1:A:829:HIS:CD2	1:A:850:CYS:HB2	2.50	0.46
1:B:1459:ASN:HD22	1:B:1460:ARG:HD2	1.80	0.46
1:B:377:THR:HA	1:B:429:THR:CG2	2.45	0.46
1:B:518:ASN:O	1:B:538:VAL:HG23	2.15	0.46
1:C:38:ALA:HB1	1:C:39:PRO:HD3	1.97	0.46
1:C:750:VAL:HG22	1:C:879:ALA:HB1	1.97	0.46
1:D:1315:HIS:CD2	1:D:1317:SER:H	2.32	0.46
1:B:92:ALA:HB3	1:B:125:GLN:HA	1.96	0.46
1:D:207:LYS:NZ	1:D:238:GLU:OE2	2.46	0.46
1:B:206:CYS:HA	1:B:312:GLU:CB	2.46	0.46
1:C:1617:VAL:HG11	1:C:1639:LEU:HD22	1.96	0.46
1:D:716:ARG:HH11	1:D:716:ARG:HG3	1.81	0.46
1:B:1537:THR:O	1:B:1541:GLU:HG2	2.16	0.46
1:B:56:GLN:O	1:B:59:ILE:HB	2.15	0.46
1:D:377:THR:HA	1:D:429:THR:CG2	2.46	0.46
1:B:1104:SER:O	1:B:1108:ARG:HG3	2.16	0.46
1:A:1469:GLN:O	1:B:64:SER:HB3	2.16	0.46
1:B:742:ARG:HD3	1:B:752:LEU:HD23	1.97	0.46
1:A:1585:VAL:HG13	1:A:1586:PHE:HD1	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1123:LEU:HD12	1:C:1183:LEU:HD23	1.98	0.46
1:C:1625:MET:HE3	1:C:1671:PHE:HZ	1.80	0.46
1:D:1085:TYR:CD1	1:D:1086:PRO:HA	2.51	0.46
1:D:1203:MET:HE1	1:D:1633:SER:HB3	1.98	0.46
1:D:600:ILE:HD11	1:D:609:TYR:CZ	2.51	0.46
1:A:1504:TYR:OH	1:B:62:SER:HB2	2.15	0.46
1:A:677:THR:OG1	1:A:680:GLU:HB2	2.16	0.46
1:A:869:PRO:HD2	1:A:872:THR:CG2	2.45	0.46
1:B:1274:GLU:HA	1:B:1277:GLU:HG3	1.98	0.46
1:B:161:VAL:HG12	1:B:187:LEU:HD22	1.98	0.46
1:D:1104:SER:O	1:D:1108:ARG:HG3	2.16	0.46
1:D:75:PRO:O	1:D:167:PRO:HD2	2.15	0.46
1:B:1085:TYR:CD1	1:B:1086:PRO:HA	2.52	0.45
1:B:125:GLN:HG2	1:B:126:PHE:CD1	2.52	0.45
1:B:1500:CYS:HB3	1:B:1504:TYR:OH	2.15	0.45
1:B:624:PHE:HD1	1:B:698:GLN:HG3	1.81	0.45
1:D:302:ARG:HB3	1:D:302:ARG:HE	1.48	0.45
1:D:624:PHE:HD1	1:D:698:GLN:HG3	1.81	0.45
1:A:1625:MET:HE3	1:A:1671:PHE:HZ	1.82	0.45
1:B:1268:ILE:HA	1:B:1271:PHE:O	2.16	0.45
1:D:1103:ASP:HA	1:D:1361:TRP:HA	1.98	0.45
1:A:1139:VAL:O	1:A:1140:ILE:HD12	2.17	0.45
1:A:1708:TRP:CE3	1:A:1709:ILE:HD12	2.50	0.45
1:B:1115:GLY:HA2	1:B:1237:PHE:HB2	1.99	0.45
1:B:1539:TYR:CD1	1:B:1610:ARG:HG2	2.52	0.45
1:C:611:GLU:C	1:C:613:ILE:H	2.20	0.45
1:D:180:VAL:HB	1:D:181:PRO:HD3	1.99	0.45
1:B:744:ILE:H	1:B:744:ILE:HG12	1.56	0.45
1:D:634:GLU:CD	1:D:1008:LYS:HE2	2.37	0.45
1:D:420:ARG:H	1:D:420:ARG:HG2	1.36	0.45
1:A:1085:TYR:CD1	1:A:1086:PRO:HA	2.51	0.45
1:A:56:GLN:O	1:A:59:ILE:HB	2.16	0.45
1:B:829:HIS:CD2	1:B:850:CYS:HB2	2.51	0.45
1:C:1057:ALA:C	1:C:1059:LYS:H	2.20	0.45
1:A:1057:ALA:C	1:A:1059:LYS:H	2.20	0.45
1:B:1625:MET:HE3	1:B:1671:PHE:CZ	2.51	0.45
1:C:1085:TYR:CD1	1:C:1086:PRO:HA	2.52	0.45
1:C:1142:VAL:HA	1:C:1182:TYR:O	2.17	0.45
1:A:1468:HIS:O	1:A:1469:GLN:C	2.53	0.45
1:A:1542:THR:O	1:D:1541:GLU:CG	2.60	0.45
1:A:1571:MET:HG2	1:A:1601:TYR:HE2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:O	1:A:41:ASP:HB3	2.16	0.45
1:B:1140:ILE:HD11	1:B:1185:ILE:HD12	1.98	0.45
1:B:1704:GLU:O	1:B:1707:ALA:HB3	2.17	0.45
1:A:1433:TYR:CE1	1:A:1502:ILE:HD13	2.52	0.45
1:D:1203:MET:CE	1:D:1633:SER:HB3	2.46	0.45
1:D:522:TYR:O	1:D:533:PRO:HA	2.17	0.45
1:D:546:ILE:HA	1:D:604:GLY:O	2.16	0.45
1:C:66:LYS:O	1:C:67:GLU:HB2	2.16	0.45
1:A:1274:GLU:HA	1:A:1277:GLU:HG3	1.99	0.45
1:A:75:PRO:O	1:A:167:PRO:HD2	2.17	0.45
1:B:1102:MET:HE1	1:B:1292:ARG:HA	1.99	0.45
1:B:521:LEU:HD23	1:B:600:ILE:CG2	2.47	0.45
1:C:194:LYS:HG2	1:C:211:CYS:SG	2.57	0.45
1:A:1259:GLY:HA3	1:A:1377:LEU:HD22	2.00	0.44
1:B:143:VAL:CG1	1:B:461:LYS:HB3	2.46	0.44
1:B:622:LYS:HE3	1:B:622:LYS:HB2	1.63	0.44
1:B:65:ASN:O	1:B:66:LYS:C	2.54	0.44
1:A:1103:ASP:OD2	1:A:1361:TRP:HB2	2.18	0.44
1:B:433:LYS:HG2	1:B:433:LYS:H	1.62	0.44
1:C:271:ASN:OD1	1:C:420:ARG:HD2	2.16	0.44
1:C:641:LYS:HB3	1:C:641:LYS:HE3	1.58	0.44
1:A:1184:SER:O	1:A:1185:ILE:HD13	2.17	0.44
1:A:75:PRO:HB2	1:A:118:ILE:HD11	1.99	0.44
1:A:828:ARG:NH2	1:A:866:PRO:O	2.43	0.44
1:B:1612:TYR:CD1	1:B:1632:GLY:HA2	2.52	0.44
1:D:1539:TYR:CD1	1:D:1610:ARG:HG2	2.52	0.44
1:D:1625:MET:HE3	1:D:1671:PHE:CZ	2.51	0.44
1:D:606:PHE:CZ	1:D:610:ILE:HD11	2.52	0.44
1:A:38:ALA:HB1	1:A:39:PRO:CD	2.48	0.44
1:C:75:PRO:O	1:C:166:VAL:HG22	2.18	0.44
1:C:66:LYS:H	1:C:66:LYS:HG3	1.55	0.44
1:B:1057:ALA:C	1:B:1059:LYS:H	2.20	0.44
1:A:641:LYS:HE3	1:A:641:LYS:HB3	1.57	0.44
1:B:141:PRO:HB2	1:B:146:ASP:HA	1.99	0.44
1:C:1274:GLU:HA	1:C:1277:GLU:HG3	1.99	0.44
1:C:1612:TYR:CD1	1:C:1632:GLY:HA2	2.52	0.44
1:D:75:PRO:O	1:D:166:VAL:HG22	2.17	0.44
1:A:283:LYS:HB2	1:A:283:LYS:HE2	1.67	0.44
1:B:634:GLU:CD	1:B:1008:LYS:HE2	2.38	0.44
1:C:1103:ASP:OD2	1:C:1361:TRP:HB2	2.18	0.44
1:C:1433:TYR:CE1	1:C:1502:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LYS:O	1:C:41:ASP:HB3	2.17	0.44
1:C:556:ASP:OD2	1:C:557:ARG:HG2	2.18	0.44
1:D:1710:ASN:O	1:D:1712:ASN:N	2.51	0.44
1:A:835:MET:HG2	1:A:933:TRP:CE3	2.53	0.44
1:B:1549:TRP:HA	1:B:1556:PHE:HB2	2.00	0.44
1:B:268:GLU:OE2	1:B:270:GLU:HB2	2.18	0.44
1:B:75:PRO:O	1:B:167:PRO:HD2	2.17	0.44
1:C:1459:ASN:HD22	1:C:1460:ARG:HD2	1.81	0.44
1:C:894:THR:HG22	1:C:895:VAL:N	2.33	0.44
1:D:1057:ALA:C	1:D:1059:LYS:H	2.22	0.44
1:A:1318:ASN:N	1:A:1318:ASN:HD22	2.16	0.44
1:A:375:VAL:HG13	1:A:401:TRP:HB3	1.99	0.44
1:A:556:ASP:OD2	1:A:557:ARG:HG2	2.18	0.44
1:C:1215:LYS:N	1:C:1218:ASP:OD2	2.41	0.44
1:C:38:ALA:HB1	1:C:39:PRO:CD	2.48	0.44
1:C:375:VAL:HG13	1:C:401:TRP:HB3	1.98	0.44
1:D:14:SER:O	1:D:18:LYS:HG2	2.17	0.44
1:B:546:ILE:HA	1:B:604:GLY:O	2.18	0.43
1:B:716:ARG:HH11	1:B:716:ARG:HG3	1.83	0.43
1:A:1468:HIS:O	1:B:62:SER:O	2.35	0.43
1:A:849:ASP:OD1	1:A:851:SER:OG	2.29	0.43
1:B:1323:VAL:HG21	1:B:1477:SER:HB3	2.00	0.43
1:B:661:SER:OG	1:B:663:HIS:ND1	2.51	0.43
1:B:78:VAL:O	1:B:120:LYS:HA	2.18	0.43
1:C:1203:MET:HE1	1:C:1633:SER:HB3	1.99	0.43
1:C:78:VAL:HG22	1:C:120:LYS:HE3	2.00	0.43
1:C:1318:ASN:HD22	1:C:1318:ASN:N	2.16	0.43
1:C:567:GLU:HG2	1:C:568:PRO:HA	1.99	0.43
1:D:862:GLU:OE1	1:D:1016:ARG:NH1	2.51	0.43
1:D:29:GLU:O	1:D:33:LYS:HG3	2.18	0.43
1:A:452:PHE:CD1	1:A:457:ARG:HG3	2.53	0.43
1:B:1103:ASP:HA	1:B:1361:TRP:HA	2.00	0.43
1:C:1140:ILE:HD11	1:C:1185:ILE:HD12	1.99	0.43
1:C:283:LYS:HE2	1:C:283:LYS:HB2	1.68	0.43
1:A:1104:SER:O	1:A:1108:ARG:HG3	2.18	0.43
1:B:78:VAL:HG22	1:B:120:LYS:HE3	2.00	0.43
1:B:1324:TYR:CZ	1:B:1347:GLY:HA3	2.53	0.43
1:B:1330:ASN:O	1:B:1336:PRO:HA	2.19	0.43
1:B:1571:MET:HG2	1:B:1601:TYR:HE2	1.83	0.43
1:C:521:LEU:HB2	1:C:546:ILE:HG12	2.00	0.43
1:D:834:MET:HG2	1:D:835:MET:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1710:ASN:O	1:A:1712:ASN:N	2.51	0.43
1:B:1617:VAL:HG11	1:B:1639:LEU:HD22	2.01	0.43
1:D:988:VAL:HA	1:D:1008:LYS:O	2.18	0.43
1:D:1323:VAL:HG21	1:D:1477:SER:HB3	2.01	0.43
1:A:715:ASP:OD2	1:A:733:ARG:NH2	2.45	0.43
1:B:1139:VAL:O	1:B:1140:ILE:HD12	2.18	0.43
1:B:75:PRO:O	1:B:166:VAL:HG22	2.19	0.43
1:B:519:TYR:HB2	1:B:546:ILE:HD13	1.99	0.43
1:C:1268:ILE:HA	1:C:1271:PHE:O	2.18	0.43
1:C:487:ALA:HB3	1:C:584:SER:HB2	1.99	0.43
1:D:1059:LYS:HD2	1:D:1059:LYS:HA	1.77	0.43
1:D:161:VAL:HG12	1:D:187:LEU:HD22	2.00	0.43
1:A:1464:GLN:O	1:A:1468:HIS:CD2	2.71	0.43
1:C:1102:MET:HE1	1:C:1292:ARG:HA	2.01	0.43
1:C:1549:TRP:HA	1:C:1556:PHE:HB2	2.01	0.43
1:D:1549:TRP:HA	1:D:1556:PHE:HB2	2.01	0.43
1:D:521:LEU:HD11	1:D:533:PRO:HB2	2.01	0.43
1:A:716:ARG:HH11	1:A:716:ARG:HG3	1.84	0.43
1:C:1540:ARG:HD2	1:C:1540:ARG:HH11	1.66	0.43
1:C:63:LYS:O	1:C:66:LYS:NZ	2.42	0.43
1:D:1142:VAL:HA	1:D:1182:TYR:O	2.19	0.43
1:D:1617:VAL:HG11	1:D:1639:LEU:HD22	2.00	0.43
1:A:7:TRP:O	1:A:167:PRO:HB3	2.19	0.43
1:A:1690:LYS:HD3	1:A:1690:LYS:HA	1.82	0.43
1:B:1123:LEU:HD12	1:B:1183:LEU:HD23	2.01	0.43
1:B:1523:LEU:HB3	1:B:1643:THR:HG21	2.01	0.43
1:B:36:LYS:HD3	1:B:36:LYS:HA	1.72	0.43
1:C:1203:MET:CE	1:C:1633:SER:HB3	2.49	0.43
1:C:1243:PRO:HB2	1:C:1246:LEU:HG	2.01	0.43
1:C:840:GLY:N	1:C:888:LYS:HG3	2.33	0.43
1:D:1730:GLU:OE2	1:D:1730:GLU:HA	2.19	0.43
1:D:268:GLU:OE2	1:D:270:GLU:HB2	2.18	0.43
1:D:437:ASP:OD1	1:D:437:ASP:N	2.52	0.43
1:B:600:ILE:HD11	1:B:609:TYR:CZ	2.54	0.42
1:B:750:VAL:HG22	1:B:879:ALA:HB1	2.00	0.42
1:C:957:ILE:CG1	1:C:1023:LEU:HD22	2.49	0.42
1:C:1710:ASN:O	1:C:1712:ASN:N	2.52	0.42
1:C:75:PRO:HB2	1:C:118:ILE:CD1	2.48	0.42
1:A:567:GLU:HG2	1:A:568:PRO:HA	2.00	0.42
1:C:1274:GLU:O	1:C:1278:GLN:HG3	2.19	0.42
1:D:1259:GLY:HA3	1:D:1377:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:VAL:CG2	1:D:163:ARG:HG3	2.49	0.42
1:D:556:ASP:HB3	1:D:557:ARG:HG2	2.01	0.42
1:D:716:ARG:HG3	1:D:716:ARG:NH1	2.34	0.42
1:A:1323:VAL:HG21	1:A:1477:SER:HB3	2.00	0.42
1:A:661:SER:OG	1:A:663:HIS:ND1	2.52	0.42
1:A:66:LYS:O	1:A:67:GLU:CB	2.67	0.42
1:C:1585:VAL:HG13	1:C:1586:PHE:CE1	2.54	0.42
1:C:661:SER:OG	1:C:663:HIS:ND1	2.51	0.42
1:C:835:MET:HG2	1:C:933:TRP:CE3	2.54	0.42
1:D:157:SER:HB3	1:D:169:SER:OG	2.18	0.42
1:A:1507:GLU:OE2	1:B:59:ILE:HG12	2.20	0.42
1:B:1102:MET:CE	1:B:1292:ARG:HA	2.50	0.42
1:C:15:PHE:HA	1:C:18:LYS:HE2	2.01	0.42
1:A:1103:ASP:HA	1:A:1361:TRP:HA	2.01	0.42
1:B:1304:TRP:CH2	1:B:1317:SER:HB3	2.54	0.42
1:C:716:ARG:HG3	1:C:716:ARG:HH11	1.85	0.42
1:D:1123:LEU:HD12	1:D:1183:LEU:HD23	2.00	0.42
1:D:66:LYS:HG3	1:D:66:LYS:H	1.59	0.42
1:A:1616:GLY:C	1:A:1642:ARG:HG3	2.40	0.42
1:A:744:ILE:H	1:A:744:ILE:HG12	1.55	0.42
1:A:81:ASN:HB3	1:A:82:ILE:HG13	2.01	0.42
1:B:1456:TYR:CZ	1:B:1460:ARG:HD3	2.54	0.42
1:C:1346:LEU:HD13	1:C:1584:ASP:HB2	2.01	0.42
1:C:180:VAL:HB	1:C:181:PRO:HD3	2.01	0.42
1:D:1243:PRO:HB2	1:D:1246:LEU:HG	2.02	0.42
1:D:1585:VAL:HG13	1:D:1586:PHE:HD1	1.77	0.42
1:D:1708:TRP:CE3	1:D:1709:ILE:HD12	2.50	0.42
1:A:1456:TYR:CZ	1:A:1460:ARG:HD3	2.55	0.42
1:B:1184:SER:O	1:B:1185:ILE:HD13	2.20	0.42
1:B:1585:VAL:HG13	1:B:1586:PHE:CE1	2.55	0.42
1:B:420:ARG:HG2	1:B:420:ARG:H	1.31	0.42
1:B:609:TYR:CZ	1:B:613:ILE:HD11	2.55	0.42
1:D:1433:TYR:CE1	1:D:1502:ILE:HD13	2.55	0.42
1:B:936:ARG:HE	1:B:936:ARG:HB3	1.64	0.42
1:A:15:PHE:CZ	1:A:27:LEU:HD22	2.55	0.42
1:A:297:LEU:HD22	1:A:404:PHE:CD1	2.55	0.42
1:A:709:GLU:HG3	1:A:914:ARG:HD3	2.02	0.42
1:A:968:LYS:HA	1:A:968:LYS:HD2	1.87	0.42
1:B:1138:THR:OG1	1:B:1139:VAL:N	2.52	0.42
1:B:1142:VAL:HA	1:B:1182:TYR:O	2.20	0.42
1:C:1456:TYR:CZ	1:C:1460:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:LYS:HA	1:D:623:PRO:HD2	1.80	0.42
1:A:224:ILE:O	1:A:228:VAL:HG23	2.20	0.42
1:A:868:LEU:HA	1:A:869:PRO:HD3	1.89	0.42
1:B:860:ILE:HG23	1:B:957:ILE:CD1	2.50	0.42
1:C:724:PHE:CE2	1:C:726:GLY:HA3	2.55	0.42
1:D:1268:ILE:HA	1:D:1271:PHE:O	2.19	0.42
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.86	0.42
1:B:207:LYS:NZ	1:B:238:GLU:OE2	2.47	0.41
1:B:420:ARG:HG2	1:B:424:LEU:O	2.20	0.41
1:B:863:THR:HG23	1:B:925:VAL:HG11	2.01	0.41
1:C:1730:GLU:OE2	1:C:1730:GLU:HA	2.20	0.41
1:D:1184:SER:O	1:D:1185:ILE:HD13	2.19	0.41
1:D:1456:TYR:CZ	1:D:1460:ARG:HD3	2.55	0.41
1:D:265:TRP:CG	1:D:272:PRO:HG3	2.54	0.41
1:A:1191:VAL:HG22	1:A:1192:PRO:HD2	2.01	0.41
1:A:1625:MET:HE3	1:A:1671:PHE:CZ	2.55	0.41
1:B:1314:LEU:HD23	1:B:1314:LEU:HA	1.88	0.41
1:C:862:GLU:OE1	1:C:1016:ARG:NH1	2.53	0.41
1:D:1654:ASP:HB3	1:D:1691:PHE:O	2.20	0.41
1:A:1102:MET:CE	1:A:1292:ARG:HA	2.50	0.41
1:A:622:LYS:HE3	1:A:622:LYS:HB2	1.67	0.41
1:D:194:LYS:HG2	1:D:211:CYS:SG	2.60	0.41
1:D:420:ARG:C	1:D:422:ASP:N	2.73	0.41
1:A:1539:TYR:CD1	1:A:1610:ARG:HG2	2.55	0.41
1:A:1549:TRP:HA	1:A:1556:PHE:HB2	2.02	0.41
1:A:1612:TYR:CD1	1:A:1632:GLY:HA2	2.55	0.41
1:B:243:PHE:CZ	1:B:435:PHE:HA	2.55	0.41
1:B:835:MET:HG2	1:B:933:TRP:HE3	1.85	0.41
1:C:1523:LEU:HB3	1:C:1643:THR:HG21	2.03	0.41
1:C:1616:GLY:C	1:C:1642:ARG:HG3	2.40	0.41
1:C:1625:MET:HE3	1:C:1671:PHE:CZ	2.55	0.41
1:C:533:PRO:HD3	1:C:606:PHE:CZ	2.55	0.41
1:D:78:VAL:O	1:D:120:LYS:HA	2.21	0.41
1:A:1268:ILE:HA	1:A:1271:PHE:O	2.19	0.41
1:A:180:VAL:HB	1:A:181:PRO:HD3	2.03	0.41
1:A:860:ILE:HG23	1:A:957:ILE:CD1	2.51	0.41
1:B:1433:TYR:CE1	1:B:1502:ILE:HD13	2.56	0.41
1:B:183:ALA:HB2	1:B:377:THR:HG21	2.03	0.41
1:D:51:GLU:H	1:D:51:GLU:CD	2.24	0.41
1:A:79:LYS:C	1:A:81:ASN:H	2.24	0.41
1:B:1523:LEU:HB3	1:B:1643:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ILE:HG23	1:B:600:ILE:O	2.21	0.41
1:B:840:GLY:N	1:B:888:LYS:HG3	2.36	0.41
1:C:1500:CYS:HB3	1:C:1504:TYR:CZ	2.55	0.41
1:C:15:PHE:HE2	1:C:24:SER:HA	1.85	0.41
1:C:270:GLU:HB3	1:C:420:ARG:HB3	2.03	0.41
1:D:1618:VAL:HG13	1:D:1625:MET:HE2	2.02	0.41
1:D:206:CYS:HA	1:D:312:GLU:CB	2.50	0.41
1:A:1151:LEU:HB3	1:A:1156:ILE:HD13	2.02	0.41
1:A:1288:TYR:CD2	1:D:1540:ARG:NH1	2.88	0.41
1:A:1556:PHE:CZ	1:A:1604:THR:HG22	2.55	0.41
1:A:14:SER:O	1:A:18:LYS:HG3	2.21	0.41
1:B:1556:PHE:CZ	1:B:1604:THR:HG22	2.56	0.41
1:B:383:LYS:HB2	1:B:386:GLU:OE1	2.20	0.41
1:B:606:PHE:CZ	1:B:610:ILE:HD11	2.56	0.41
1:C:1103:ASP:HA	1:C:1361:TRP:HA	2.02	0.41
1:C:1459:ASN:HD21	1:C:1460:ARG:NH1	2.03	0.41
1:D:1612:TYR:CD1	1:D:1632:GLY:HA2	2.56	0.41
1:D:840:GLY:N	1:D:888:LYS:HG3	2.36	0.41
1:A:16:HIS:ND1	1:A:24:SER:HB2	2.36	0.41
1:A:635:ILE:HA	1:A:635:ILE:HD12	1.88	0.41
1:B:1466:GLU:O	1:B:1469:GLN:N	2.52	0.41
1:D:1152:ASN:O	1:D:1153:ASP:HB2	2.20	0.41
1:D:1304:TRP:CG	1:D:1316:PRO:HB2	2.56	0.41
1:A:1314:LEU:HA	1:A:1314:LEU:HD23	1.88	0.41
1:B:868:LEU:HA	1:B:869:PRO:HD3	1.90	0.41
1:C:1184:SER:O	1:C:1185:ILE:HD13	2.20	0.41
1:C:1323:VAL:HG21	1:C:1477:SER:HB3	2.02	0.41
1:C:296:PRO:HG2	1:C:366:LEU:HD22	2.03	0.41
1:C:81:ASN:HB3	1:C:82:ILE:HG13	2.02	0.41
1:D:968:LYS:HD2	1:D:968:LYS:HA	1.90	0.41
1:A:1274:GLU:O	1:A:1278:GLN:HG3	2.20	0.41
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.89	0.41
1:B:51:GLU:H	1:B:51:GLU:CD	2.24	0.41
1:C:1539:TYR:CD1	1:C:1610:ARG:HG2	2.56	0.41
1:C:143:VAL:HG13	1:C:461:LYS:HB3	2.02	0.41
1:C:69:LEU:HA	1:C:69:LEU:HD23	1.90	0.41
1:D:516:SER:O	1:D:518:ASN:N	2.52	0.41
1:D:701:ILE:HA	1:D:702:PRO:HD3	1.92	0.41
1:D:750:VAL:HG22	1:D:879:ALA:HB1	2.02	0.41
1:D:753:VAL:HA	1:D:754:PRO:HD3	1.95	0.41
1:B:1468:HIS:O	1:B:1469:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:ASN:HD21	1:B:1601:TYR:HB3	1.86	0.41
1:B:751:PRO:O	1:B:907:TYR:HA	2.21	0.41
1:C:1269:ASP:OD2	1:C:1269:ASP:N	2.47	0.41
1:C:81:ASN:O	1:C:203:VAL:HG13	2.21	0.41
1:C:85:LYS:HD3	1:D:1509:GLN:HE22	1.85	0.41
1:C:860:ILE:HG23	1:C:957:ILE:CD1	2.50	0.41
1:D:1139:VAL:O	1:D:1140:ILE:HD12	2.20	0.41
1:D:851:SER:O	1:D:1058:THR:HA	2.21	0.41
1:A:1469:GLN:CB	1:B:64:SER:H	2.34	0.40
1:A:1:MET:HB2	1:A:2:GLU:H	1.59	0.40
1:C:1524:PRO:O	1:C:1643:THR:HG23	2.22	0.40
1:C:524:LEU:HB2	1:C:532:LYS:O	2.20	0.40
1:C:737:LEU:HB2	1:C:740:SER:OG	2.21	0.40
1:C:90:THR:HG22	1:C:92:ALA:N	2.32	0.40
1:D:1138:THR:OG1	1:D:1139:VAL:N	2.54	0.40
1:A:1194:TYR:CE2	1:A:1206:MET:HG2	2.56	0.40
1:A:78:VAL:HG23	1:A:82:ILE:HB	2.02	0.40
1:B:1151:LEU:HB3	1:B:1156:ILE:HD13	2.04	0.40
1:B:724:PHE:CE2	1:B:726:GLY:HA3	2.56	0.40
1:C:1151:LEU:HB3	1:C:1156:ILE:HD13	2.02	0.40
1:C:894:THR:O	1:C:911:VAL:HG13	2.21	0.40
1:D:1523:LEU:HB3	1:D:1643:THR:HG21	2.03	0.40
1:A:1006:LEU:HD23	1:A:1006:LEU:HA	1.96	0.40
1:A:1085:TYR:CE2	1:A:1108:ARG:HD3	2.56	0.40
1:A:1730:GLU:HA	1:A:1730:GLU:OE2	2.21	0.40
1:B:1191:VAL:HG22	1:B:1192:PRO:HD2	2.04	0.40
1:C:375:VAL:HG13	1:C:376:PRO:O	2.21	0.40
1:C:75:PRO:O	1:C:167:PRO:HD2	2.21	0.40
1:D:1085:TYR:CE2	1:D:1108:ARG:HD3	2.56	0.40
1:D:1302:PRO:HG3	1:D:1331:PHE:CE2	2.56	0.40
1:D:1391:LYS:HA	1:D:1391:LYS:HD2	1.93	0.40
1:D:1459:ASN:HD21	1:D:1460:ARG:NH1	2.04	0.40
1:A:925:VAL:HG23	1:A:926:THR:HG23	2.04	0.40
1:B:1730:GLU:HA	1:B:1730:GLU:OE2	2.20	0.40
1:C:36:LYS:HD3	1:C:40:GLU:CD	2.42	0.40
1:C:622:LYS:HE3	1:C:622:LYS:HB2	1.71	0.40
1:B:1151:LEU:HD11	1:B:1168:ASP:HB3	2.04	0.40
1:B:157:SER:HB3	1:B:169:SER:OG	2.21	0.40
1:B:519:TYR:CB	1:B:546:ILE:HD13	2.52	0.40
1:C:1059:LYS:HD2	1:C:1059:LYS:HA	1.75	0.40
1:D:1468:HIS:O	1:D:1469:GLN:C	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:ILE:HG23	1:D:957:ILE:CD1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:TYR:OH	1:C:1541:GLU:OE2[2_455]	1.97	0.23

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1654/1829 (90%)	1540 (93%)	101 (6%)	13 (1%)	22	66
1	B	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	25	68
1	C	1654/1829 (90%)	1539 (93%)	102 (6%)	13 (1%)	22	66
1	D	1652/1829 (90%)	1544 (94%)	97 (6%)	11 (1%)	25	68
All	All	6612/7316 (90%)	6167 (93%)	397 (6%)	48 (1%)	25	68

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	1166	ARG
1	A	1711	GLU
1	B	1166	ARG
1	C	38	ALA
1	C	1166	ARG
1	C	1711	GLU
1	D	1166	ARG
1	D	1711	GLU

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Mol	Chain	Res	Type
1	A	206	CYS
1	A	479	ASP
1	A	1438	ASP
1	B	206	CYS
1	B	479	ASP
1	B	540	ASP
1	B	1438	ASP
1	C	206	CYS
1	C	479	ASP
1	C	1438	ASP
1	D	206	CYS
1	D	479	ASP
1	D	540	ASP
1	D	1438	ASP
1	A	891	CYS
1	B	104	SER
1	B	891	CYS
1	C	891	CYS
1	D	104	SER
1	D	891	CYS
1	A	104	SER
1	A	517	ASN
1	A	612	HIS
1	C	104	SER
1	C	517	ASN
1	C	612	HIS
1	A	1003	ASP
1	A	1058	THR
1	B	65	ASN
1	B	1003	ASP
1	C	1003	ASP
1	C	1058	THR
1	D	1003	ASP
1	D	1058	THR
1	B	1058	THR
1	A	37	PRO
1	C	37	PRO
1	B	37	PRO
1	D	37	PRO

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	1413/1547 (91%)	1275 (90%)	138 (10%)	9	34
1	B	1411/1547 (91%)	1264 (90%)	147 (10%)	8	32
1	C	1413/1547 (91%)	1274 (90%)	139 (10%)	9	34
1	D	1411/1547 (91%)	1263 (90%)	148 (10%)	8	32
All	All	5648/6188 (91%)	5076 (90%)	572 (10%)	9	33

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	4	THR
1	A	18	LYS
1	A	60	LEU
1	A	62	SER
1	A	66	LYS
1	A	67	GLU
1	A	78	VAL
1	A	90	THR
1	A	95	SER
1	A	106	VAL
1	A	116	VAL
1	A	121	THR
1	A	143	VAL
1	A	149	VAL
1	A	160	VAL
1	A	165	ILE
1	A	166	VAL
1	A	170	LEU
1	A	194	LYS
1	A	202	VAL
1	A	219	LEU
1	A	231	LYS

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Mol	Chain	Res	Type
1	A	241	ARG
1	A	243	PHE
1	A	269	THR
1	A	283	LYS
1	A	305	TYR
1	A	310	VAL
1	A	323	THR
1	A	343	LYS
1	A	356	ARG
1	A	368	LYS
1	A	375	VAL
1	A	385	GLU
1	A	393	LEU
1	A	415	VAL
1	A	420	ARG
1	A	429	THR
1	A	434	LYS
1	A	437	ASP
1	A	445	LYS
1	A	463	VAL
1	A	540	ASP
1	A	547	GLN
1	A	582	VAL
1	A	593	THR
1	A	600	ILE
1	A	631	ASN
1	A	634	GLU
1	A	638	ARG
1	A	659	LYS
1	A	662	GLN
1	A	676	ARG
1	A	680	GLU
1	A	689	ILE
1	A	698	GLN
1	A	716	ARG
1	A	719	GLN
1	A	730	ASP
1	A	734	LYS
1	A	735	LEU
1	A	737	LEU
1	A	738	LYS
1	A	739	HIS

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Mol	Chain	Res	Type
1	A	743	GLU
1	A	744	ILE
1	A	746	GLU
1	A	752	LEU
1	A	834	MET
1	A	841	LYS
1	A	859	VAL
1	A	860	ILE
1	A	872	THR
1	A	875	LYS
1	A	888	LYS
1	A	944	ASP
1	A	951	GLU
1	A	952	VAL
1	A	957	ILE
1	A	978	THR
1	A	979	SER
1	A	988	VAL
1	A	999	SER
1	A	1011	VAL
1	A	1015	ASP
1	A	1016	ARG
1	A	1042	LEU
1	A	1044	SER
1	A	1047	SER
1	A	1055	LYS
1	A	1067	LYS
1	A	1074	LEU
1	A	1079	ASN
1	A	1103	ASP
1	A	1131	LYS
1	A	1147	VAL
1	A	1150	THR
1	A	1171	SER
1	A	1172	VAL
1	A	1191	VAL
1	A	1216	LEU
1	A	1224	GLN
1	A	1227	LEU
1	A	1252	THR
1	A	1311	GLU
1	A	1321	ASP

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Mol	Chain	Res	Type
1	A	1326	LEU
1	A	1345	SER
1	A	1346	LEU
1	A	1375	VAL
1	A	1388	SER
1	A	1393	ILE
1	A	1396	PHE
1	A	1402	LEU
1	A	1408	LYS
1	A	1426	ASP
1	A	1428	SER
1	A	1430	LYS
1	A	1440	TYR
1	A	1459	ASN
1	A	1460	ARG
1	A	1478	GLN
1	A	1516	VAL
1	A	1562	ASP
1	A	1565	ARG
1	A	1571	MET
1	A	1585	VAL
1	A	1625	MET
1	A	1643	THR
1	A	1662	LEU
1	A	1675	THR
1	A	1695	VAL
1	A	1697	GLU
1	A	1721	GLU
1	A	1726	GLU
1	A	1736	GLN
1	B	4	THR
1	B	23	LYS
1	B	25	LEU
1	B	27	LEU
1	B	31	LEU
1	B	66	LYS
1	B	78	VAL
1	B	81	ASN
1	B	90	THR
1	B	95	SER
1	B	106	VAL
1	B	116	VAL

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Mol	Chain	Res	Type
1	B	118	ILE
1	B	121	THR
1	B	160	VAL
1	B	166	VAL
1	B	170	LEU
1	B	184	LEU
1	B	191	LYS
1	B	194	LYS
1	B	202	VAL
1	B	217	LEU
1	B	219	LEU
1	B	220	SER
1	B	241	ARG
1	B	243	PHE
1	B	277	LYS
1	B	302	ARG
1	B	305	TYR
1	B	313	ARG
1	B	317	THR
1	B	345	ASP
1	B	351	LYS
1	B	368	LYS
1	B	369	ASP
1	B	375	VAL
1	B	393	LEU
1	B	420	ARG
1	B	428	ILE
1	B	429	THR
1	B	433	LYS
1	B	437	ASP
1	B	445	LYS
1	B	463	VAL
1	B	468	THR
1	B	517	ASN
1	B	518	ASN
1	B	526	LYS
1	B	536	ARG
1	B	537	ARG
1	B	538	VAL
1	B	542	THR
1	B	582	VAL
1	B	584	SER

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Mol	Chain	Res	Type
1	B	589	GLU
1	B	593	THR
1	B	600	ILE
1	B	631	ASN
1	B	634	GLU
1	B	638	ARG
1	B	659	LYS
1	B	662	GLN
1	B	676	ARG
1	B	680	GLU
1	B	689	ILE
1	B	698	GLN
1	B	716	ARG
1	B	719	GLN
1	B	730	ASP
1	B	734	LYS
1	B	735	LEU
1	B	737	LEU
1	B	738	LYS
1	B	739	HIS
1	B	743	GLU
1	B	744	ILE
1	B	746	GLU
1	B	752	LEU
1	B	834	MET
1	B	841	LYS
1	B	859	VAL
1	B	860	ILE
1	B	872	THR
1	B	875	LYS
1	B	888	LYS
1	B	944	ASP
1	B	951	GLU
1	B	952	VAL
1	B	957	ILE
1	B	978	THR
1	B	979	SER
1	B	988	VAL
1	B	999	SER
1	B	1011	VAL
1	B	1015	ASP
1	B	1016	ARG

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Mol	Chain	Res	Type
1	B	1042	LEU
1	B	1044	SER
1	B	1047	SER
1	B	1055	LYS
1	B	1067	LYS
1	B	1074	LEU
1	B	1079	ASN
1	B	1103	ASP
1	B	1131	LYS
1	B	1147	VAL
1	B	1150	THR
1	B	1171	SER
1	B	1172	VAL
1	B	1191	VAL
1	B	1216	LEU
1	B	1224	GLN
1	B	1227	LEU
1	B	1252	THR
1	B	1303	LYS
1	B	1311	GLU
1	B	1321	ASP
1	B	1326	LEU
1	B	1345	SER
1	B	1346	LEU
1	B	1375	VAL
1	B	1388	SER
1	B	1393	ILE
1	B	1396	PHE
1	B	1402	LEU
1	B	1408	LYS
1	B	1426	ASP
1	B	1428	SER
1	B	1430	LYS
1	B	1440	TYR
1	B	1459	ASN
1	B	1460	ARG
1	B	1478	GLN
1	B	1516	VAL
1	B	1562	ASP
1	B	1565	ARG
1	B	1571	MET
1	B	1585	VAL

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Mol	Chain	Res	Type
1	B	1625	MET
1	B	1643	THR
1	B	1662	LEU
1	B	1675	THR
1	B	1695	VAL
1	B	1697	GLU
1	B	1721	GLU
1	B	1726	GLU
1	B	1736	GLN
1	C	1	MET
1	C	2	GLU
1	C	4	THR
1	C	18	LYS
1	C	60	LEU
1	C	62	SER
1	C	66	LYS
1	C	67	GLU
1	C	78	VAL
1	C	90	THR
1	C	95	SER
1	C	106	VAL
1	C	116	VAL
1	C	121	THR
1	C	123	LEU
1	C	143	VAL
1	C	160	VAL
1	C	165	ILE
1	C	166	VAL
1	C	170	LEU
1	C	194	LYS
1	C	202	VAL
1	C	219	LEU
1	C	231	LYS
1	C	241	ARG
1	C	243	PHE
1	C	269	THR
1	C	283	LYS
1	C	305	TYR
1	C	310	VAL
1	C	323	THR
1	C	343	LYS
1	C	356	ARG

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Mol	Chain	Res	Type
1	C	368	LYS
1	C	375	VAL
1	C	385	GLU
1	C	393	LEU
1	C	415	VAL
1	C	420	ARG
1	C	429	THR
1	C	434	LYS
1	C	437	ASP
1	C	445	LYS
1	C	463	VAL
1	C	466	ARG
1	C	540	ASP
1	C	547	GLN
1	C	582	VAL
1	C	593	THR
1	C	600	ILE
1	C	631	ASN
1	C	634	GLU
1	C	638	ARG
1	C	659	LYS
1	C	662	GLN
1	C	676	ARG
1	C	680	GLU
1	C	689	ILE
1	C	698	GLN
1	C	716	ARG
1	C	719	GLN
1	C	730	ASP
1	C	734	LYS
1	C	735	LEU
1	C	737	LEU
1	C	738	LYS
1	C	739	HIS
1	C	743	GLU
1	C	744	ILE
1	C	746	GLU
1	C	752	LEU
1	C	834	MET
1	C	841	LYS
1	C	859	VAL
1	C	860	ILE

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Mol	Chain	Res	Type
1	C	872	THR
1	C	875	LYS
1	C	888	LYS
1	C	944	ASP
1	C	951	GLU
1	C	952	VAL
1	C	957	ILE
1	C	978	THR
1	C	979	SER
1	C	988	VAL
1	C	999	SER
1	C	1011	VAL
1	C	1015	ASP
1	C	1016	ARG
1	C	1042	LEU
1	C	1044	SER
1	C	1047	SER
1	C	1055	LYS
1	C	1067	LYS
1	C	1074	LEU
1	C	1079	ASN
1	C	1103	ASP
1	C	1131	LYS
1	C	1147	VAL
1	C	1150	THR
1	C	1171	SER
1	C	1172	VAL
1	C	1191	VAL
1	C	1216	LEU
1	C	1224	GLN
1	C	1227	LEU
1	C	1252	THR
1	C	1311	GLU
1	C	1321	ASP
1	C	1326	LEU
1	C	1345	SER
1	C	1346	LEU
1	C	1375	VAL
1	C	1388	SER
1	C	1393	ILE
1	C	1396	PHE
1	C	1402	LEU

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Mol	Chain	Res	Type
1	C	1408	LYS
1	C	1426	ASP
1	C	1428	SER
1	C	1430	LYS
1	C	1440	TYR
1	C	1459	ASN
1	C	1460	ARG
1	C	1478	GLN
1	C	1516	VAL
1	C	1562	ASP
1	C	1565	ARG
1	C	1571	MET
1	C	1585	VAL
1	C	1625	MET
1	C	1643	THR
1	C	1662	LEU
1	C	1675	THR
1	C	1695	VAL
1	C	1697	GLU
1	C	1721	GLU
1	C	1726	GLU
1	C	1736	GLN
1	D	4	THR
1	D	23	LYS
1	D	25	LEU
1	D	27	LEU
1	D	31	LEU
1	D	66	LYS
1	D	78	VAL
1	D	81	ASN
1	D	90	THR
1	D	95	SER
1	D	106	VAL
1	D	116	VAL
1	D	118	ILE
1	D	121	THR
1	D	143	VAL
1	D	160	VAL
1	D	166	VAL
1	D	170	LEU
1	D	184	LEU
1	D	191	LYS

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Mol	Chain	Res	Type
1	D	194	LYS
1	D	202	VAL
1	D	217	LEU
1	D	219	LEU
1	D	220	SER
1	D	241	ARG
1	D	243	PHE
1	D	277	LYS
1	D	302	ARG
1	D	305	TYR
1	D	313	ARG
1	D	317	THR
1	D	345	ASP
1	D	351	LYS
1	D	368	LYS
1	D	369	ASP
1	D	375	VAL
1	D	393	LEU
1	D	420	ARG
1	D	428	ILE
1	D	429	THR
1	D	433	LYS
1	D	437	ASP
1	D	445	LYS
1	D	458	THR
1	D	463	VAL
1	D	468	THR
1	D	517	ASN
1	D	518	ASN
1	D	526	LYS
1	D	536	ARG
1	D	537	ARG
1	D	538	VAL
1	D	542	THR
1	D	582	VAL
1	D	584	SER
1	D	589	GLU
1	D	593	THR
1	D	600	ILE
1	D	631	ASN
1	D	634	GLU
1	D	638	ARG

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Mol	Chain	Res	Type
1	D	659	LYS
1	D	662	GLN
1	D	676	ARG
1	D	680	GLU
1	D	689	ILE
1	D	698	GLN
1	D	716	ARG
1	D	719	GLN
1	D	730	ASP
1	D	734	LYS
1	D	735	LEU
1	D	737	LEU
1	D	738	LYS
1	D	739	HIS
1	D	743	GLU
1	D	744	ILE
1	D	746	GLU
1	D	752	LEU
1	D	834	MET
1	D	841	LYS
1	D	859	VAL
1	D	860	ILE
1	D	872	THR
1	D	875	LYS
1	D	888	LYS
1	D	944	ASP
1	D	951	GLU
1	D	952	VAL
1	D	957	ILE
1	D	978	THR
1	D	979	SER
1	D	988	VAL
1	D	999	SER
1	D	1011	VAL
1	D	1015	ASP
1	D	1016	ARG
1	D	1042	LEU
1	D	1044	SER
1	D	1047	SER
1	D	1055	LYS
1	D	1067	LYS
1	D	1074	LEU

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Mol	Chain	Res	Type
1	D	1079	ASN
1	D	1103	ASP
1	D	1131	LYS
1	D	1147	VAL
1	D	1150	THR
1	D	1171	SER
1	D	1172	VAL
1	D	1191	VAL
1	D	1216	LEU
1	D	1224	GLN
1	D	1227	LEU
1	D	1252	THR
1	D	1311	GLU
1	D	1321	ASP
1	D	1326	LEU
1	D	1345	SER
1	D	1346	LEU
1	D	1375	VAL
1	D	1388	SER
1	D	1393	ILE
1	D	1396	PHE
1	D	1402	LEU
1	D	1408	LYS
1	D	1426	ASP
1	D	1428	SER
1	D	1430	LYS
1	D	1440	TYR
1	D	1459	ASN
1	D	1460	ARG
1	D	1478	GLN
1	D	1516	VAL
1	D	1562	ASP
1	D	1565	ARG
1	D	1571	MET
1	D	1585	VAL
1	D	1625	MET
1	D	1643	THR
1	D	1662	LEU
1	D	1675	THR
1	D	1695	VAL
1	D	1697	GLU
1	D	1721	GLU

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Mol	Chain	Res	Type
1	D	1726	GLU
1	D	1736	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	81	ASN
1	A	186	ASN
1	A	829	HIS
1	A	1459	ASN
1	B	99	GLN
1	B	186	ASN
1	B	539	ASN
1	B	829	HIS
1	B	1315	HIS
1	B	1318	ASN
1	B	1459	ASN
1	C	55	HIS
1	C	58	ASN
1	C	65	ASN
1	C	81	ASN
1	C	186	ASN
1	C	829	HIS
1	C	1459	ASN
1	C	1468	HIS
1	C	1509	GLN
1	D	99	GLN
1	D	186	ASN
1	D	539	ASN
1	D	829	HIS
1	D	1315	HIS
1	D	1318	ASN
1	D	1459	ASN
1	D	1468	HIS
1	D	1509	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1660/1829 (90%)	0.49	127 (7%)	14	20	236, 291, 352, 387	0
1	B	1658/1829 (90%)	0.43	99 (5%)	23	26	245, 295, 361, 403	0
1	C	1660/1829 (90%)	0.54	149 (8%)	10	17	269, 323, 368, 413	0
1	D	1658/1829 (90%)	0.49	110 (6%)	19	23	254, 306, 345, 377	0
All	All	6636/7316 (90%)	0.49	485 (7%)	16	21	236, 307, 356, 413	0

All (485) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1736	GLN	7.4
1	C	1626	CYS	6.7
1	C	189	GLY	6.7
1	C	1226	GLU	6.7
1	C	1619	GLY	5.8
1	D	972	PRO	5.6
1	D	1736	GLN	5.5
1	C	570	GLY	5.4
1	C	177	SER	5.3
1	C	572	GLY	5.3
1	A	1226	GLU	5.3
1	B	570	GLY	5.2
1	B	177	SER	5.0
1	A	177	SER	4.9
1	D	572	GLY	4.8
1	C	916	GLN	4.8
1	C	167	PRO	4.8
1	D	1619	GLY	4.8
1	A	916	GLN	4.8
1	A	949	LYS	4.7
1	C	1637	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	570	GLY	4.7
1	C	153	SER	4.7
1	A	1001	GLU	4.6
1	A	570	GLY	4.6
1	A	1225	PRO	4.6
1	A	154	SER	4.6
1	D	177	SER	4.5
1	A	216	ALA	4.4
1	A	1223	ASN	4.4
1	C	176	GLY	4.4
1	A	183	ALA	4.4
1	C	1604	THR	4.4
1	B	572	GLY	4.3
1	C	605	GLY	4.3
1	C	1621	GLY	4.2
1	C	129	GLY	4.2
1	C	307	GLY	4.2
1	C	751	PRO	4.2
1	D	916	GLN	4.2
1	B	573	SER	4.2
1	B	1736	GLN	4.1
1	A	167	PRO	4.1
1	C	157	SER	4.1
1	D	914	ARG	4.1
1	A	703	GLY	4.1
1	D	1223	ASN	4.1
1	A	1622	GLY	4.1
1	A	572	GLY	4.0
1	A	1228	SER	4.0
1	A	1658	ASP	4.0
1	A	918	GLU	4.0
1	A	573	SER	3.9
1	A	169	SER	3.9
1	D	1626	CYS	3.9
1	A	604	GLY	3.9
1	B	176	GLY	3.9
1	A	426	ASN	3.9
1	C	306	GLU	3.9
1	C	918	GLU	3.9
1	A	1736	GLN	3.8
1	A	1547	ALA	3.8
1	B	1622	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	971	ARG	3.8
1	C	1403	GLU	3.8
1	C	175	ALA	3.8
1	D	425	PRO	3.8
1	D	1397	GLU	3.8
1	A	307	GLY	3.8
1	A	1619	GLY	3.8
1	C	169	SER	3.7
1	C	1732	ALA	3.7
1	D	1226	GLU	3.7
1	A	1	MET	3.7
1	B	1548	PRO	3.7
1	D	167	PRO	3.7
1	A	734	LYS	3.7
1	A	736	GLY	3.6
1	C	1282	ASP	3.6
1	C	178	GLY	3.6
1	A	826	ASN	3.6
1	C	1622	GLY	3.6
1	A	1626	CYS	3.6
1	B	153	SER	3.5
1	C	1438	ASP	3.5
1	C	308	ALA	3.5
1	A	676	ARG	3.5
1	B	916	GLN	3.5
1	C	1471	VAL	3.5
1	D	169	SER	3.5
1	A	129	GLY	3.5
1	A	2	GLU	3.5
1	C	1603	GLY	3.5
1	B	914	ARG	3.5
1	C	414	ALA	3.4
1	B	1303	LYS	3.4
1	B	129	GLY	3.4
1	D	153	SER	3.4
1	A	1230	SER	3.4
1	D	122	ASN	3.4
1	C	468	THR	3.4
1	C	1188	GLY	3.4
1	B	947	ASN	3.4
1	D	424	LEU	3.4
1	B	838	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	468	THR	3.3
1	B	1190	ASP	3.3
1	D	1400	SER	3.3
1	A	652	ALA	3.3
1	A	1548	PRO	3.3
1	D	1560	VAL	3.3
1	A	171	GLY	3.3
1	A	545	GLN	3.3
1	C	154	SER	3.3
1	A	1591	CYS	3.3
1	A	1188	GLY	3.3
1	A	1224	GLN	3.3
1	B	427	GLY	3.3
1	C	1000	ALA	3.3
1	C	1437	GLY	3.2
1	A	1229	VAL	3.2
1	C	908	PHE	3.2
1	C	152	GLY	3.2
1	B	1623	MET	3.2
1	D	1697	GLU	3.2
1	C	831	GLU	3.2
1	B	1188	GLY	3.1
1	B	1619	GLY	3.1
1	A	914	ARG	3.1
1	C	1426	ASP	3.1
1	C	753	VAL	3.1
1	B	944	ASP	3.1
1	C	999	SER	3.1
1	C	1737	VAL	3.1
1	B	520	LYS	3.1
1	C	1190	ASP	3.1
1	C	1321	ASP	3.1
1	D	1399	GLY	3.1
1	C	1427	LEU	3.1
1	A	1000	ALA	3.1
1	A	213	SER	3.1
1	A	178	GLY	3.1
1	C	942	SER	3.1
1	A	182	ALA	3.1
1	C	1724	GLY	3.1
1	D	912	ASN	3.1
1	B	1542	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	1732	ALA	3.0
1	A	425	PRO	3.0
1	C	213	SER	3.0
1	C	1677	GLU	3.0
1	D	1735	ILE	3.0
1	D	242	GLU	3.0
1	C	1314	LEU	3.0
1	A	427	GLY	3.0
1	D	1607	ASN	3.0
1	A	157	SER	3.0
1	D	1000	ALA	3.0
1	B	169	SER	3.0
1	C	621	LYS	3.0
1	A	377	THR	3.0
1	A	1282	ASP	3.0
1	B	1626	CYS	3.0
1	C	943	PRO	3.0
1	D	381	ASN	3.0
1	D	426	ASN	3.0
1	B	171	GLY	2.9
1	C	183	ALA	2.9
1	C	1697	GLU	2.9
1	D	1187	GLY	2.9
1	A	1592	ALA	2.9
1	C	912	ASN	2.9
1	C	174	THR	2.9
1	C	754	PRO	2.9
1	C	1623	MET	2.9
1	B	1550	LEU	2.9
1	B	242	GLU	2.9
1	A	1321	ASP	2.9
1	A	587	CYS	2.9
1	B	837	ASP	2.9
1	C	1356	ALA	2.9
1	C	604	GLY	2.8
1	D	542	THR	2.8
1	D	1548	PRO	2.8
1	A	153	SER	2.8
1	D	1395	ASN	2.8
1	C	469	VAL	2.8
1	C	1624	TYR	2.8
1	D	128	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	1584	ASP	2.8
1	B	1226	GLU	2.8
1	D	702	PRO	2.8
1	B	948	THR	2.8
1	C	1320	HIS	2.8
1	D	427	GLY	2.8
1	A	1737	VAL	2.8
1	A	1697	GLU	2.8
1	B	1278	GLN	2.8
1	A	381	ASN	2.8
1	D	173	ASP	2.8
1	D	631	ASN	2.8
1	C	1230	SER	2.8
1	B	1012	HIS	2.8
1	D	676	ARG	2.8
1	C	461	LYS	2.7
1	B	912	ASN	2.7
1	C	122	ASN	2.7
1	D	1334	ASP	2.7
1	C	894	THR	2.7
1	D	1314	LEU	2.7
1	B	1677	GLU	2.7
1	B	1236	ASP	2.7
1	D	138	GLY	2.7
1	B	1591	CYS	2.7
1	C	125	GLN	2.7
1	A	145	ASN	2.7
1	B	1547	ALA	2.7
1	A	893	GLY	2.7
1	A	1535	CYS	2.7
1	C	1560	VAL	2.7
1	A	303	CYS	2.7
1	D	1315	HIS	2.7
1	D	893	GLY	2.7
1	C	1228	SER	2.7
1	D	216	ALA	2.7
1	A	1320	HIS	2.7
1	C	1723	GLN	2.7
1	C	861	GLU	2.7
1	C	1229	VAL	2.7
1	B	414	ALA	2.6
1	C	1225	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	2.6
1	A	999	SER	2.6
1	B	855	ARG	2.6
1	D	1328	ALA	2.6
1	C	1633	SER	2.6
1	D	1592	ALA	2.6
1	C	173	ASP	2.6
1	D	655	SER	2.6
1	B	1116	ASN	2.6
1	C	1735	ILE	2.6
1	A	1062	ASP	2.6
1	C	1566	ASN	2.6
1	A	75	PRO	2.6
1	D	1224	GLN	2.6
1	B	1621	GLY	2.6
1	A	1604	THR	2.6
1	C	171	GLY	2.6
1	C	584	SER	2.6
1	A	1581	GLY	2.6
1	A	1550	LEU	2.6
1	C	826	ASN	2.6
1	C	1223	ASN	2.6
1	D	866	PRO	2.6
1	D	1622	GLY	2.6
1	B	1413	TYR	2.5
1	D	64	SER	2.5
1	A	947	ASN	2.5
1	B	918	GLU	2.5
1	B	949	LYS	2.5
1	A	1711	GLU	2.5
1	A	731	ALA	2.5
1	C	417	SER	2.5
1	A	1603	GLY	2.5
1	B	1275	TYR	2.5
1	C	1592	ALA	2.5
1	D	1680	GLU	2.5
1	A	595	GLN	2.5
1	A	651	VAL	2.5
1	A	1233	PRO	2.5
1	B	1353	ALA	2.5
1	C	427	GLY	2.5
1	D	1303	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	751	PRO	2.4
1	C	848	ARG	2.4
1	B	421	SER	2.4
1	C	907	TYR	2.4
1	C	941	ASP	2.4
1	C	1227	LEU	2.4
1	C	906	PHE	2.4
1	D	523	ALA	2.4
1	A	215	PHE	2.4
1	A	1002	TYR	2.4
1	C	1472	GLY	2.4
1	C	397	ARG	2.4
1	A	46	SER	2.4
1	B	749	LYS	2.4
1	B	183	ALA	2.4
1	B	1321	ASP	2.4
1	A	1187	GLY	2.4
1	B	1603	GLY	2.4
1	A	1358	ALA	2.4
1	B	951	GLU	2.4
1	C	1312	ALA	2.4
1	B	1237	PHE	2.4
1	C	1591	CYS	2.4
1	D	1437	GLY	2.4
1	B	969	ASP	2.4
1	A	695	THR	2.4
1	C	850	CYS	2.4
1	C	1319	ALA	2.4
1	B	1187	GLY	2.4
1	B	1658	ASP	2.4
1	C	1548	PRO	2.4
1	D	1547	ALA	2.4
1	A	740	SER	2.4
1	D	1569	LYS	2.4
1	D	148	TYR	2.4
1	D	1438	ASP	2.4
1	C	601	THR	2.4
1	C	1658	ASP	2.4
1	D	1261	THR	2.4
1	A	722	ILE	2.3
1	A	379	PRO	2.3
1	B	1584	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1315	HIS	2.3
1	D	1190	ASP	2.3
1	A	749	LYS	2.3
1	B	831	GLU	2.3
1	A	1231	SER	2.3
1	C	1234	ALA	2.3
1	D	861	GLU	2.3
1	A	1584	ASP	2.3
1	B	1732	ALA	2.3
1	A	670	SER	2.3
1	C	742	ARG	2.3
1	C	182	ALA	2.3
1	D	92	ALA	2.3
1	C	1236	ASP	2.3
1	C	1482	SER	2.3
1	A	1637	TYR	2.3
1	C	1680	GLU	2.3
1	A	855	ARG	2.3
1	C	416	PRO	2.3
1	C	1574	SER	2.3
1	B	1358	ALA	2.3
1	B	1311	GLU	2.3
1	A	523	ALA	2.3
1	D	140	THR	2.3
1	B	429	THR	2.3
1	D	1636	GLY	2.3
1	B	213	SER	2.3
1	B	243	PHE	2.3
1	B	1544	ARG	2.3
1	C	497	PRO	2.3
1	C	1103	ASP	2.3
1	A	1532	THR	2.3
1	C	586	ILE	2.3
1	D	137	TYR	2.3
1	C	1091	TYR	2.3
1	A	148	TYR	2.3
1	A	831	GLU	2.3
1	C	75	PRO	2.3
1	D	1225	PRO	2.3
1	D	633	GLY	2.3
1	B	1223	ASN	2.3
1	A	737	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	709	GLU	2.2
1	C	914	ARG	2.2
1	B	741	ALA	2.2
1	B	1352	GLN	2.2
1	A	917	VAL	2.2
1	A	1227	LEU	2.2
1	A	1334	ASP	2.2
1	D	1282	ASP	2.2
1	B	1184	SER	2.2
1	A	605	GLY	2.2
1	A	1621	GLY	2.2
1	B	198	SER	2.2
1	B	1546	GLU	2.2
1	C	1011	VAL	2.2
1	C	1231	SER	2.2
1	C	1313	GLY	2.2
1	D	1354	VAL	2.2
1	D	83	ASP	2.2
1	D	135	SER	2.2
1	D	894	THR	2.2
1	D	1677	GLU	2.2
1	B	1320	HIS	2.2
1	A	702	PRO	2.2
1	D	1603	GLY	2.2
1	A	173	ASP	2.2
1	D	421	SER	2.2
1	D	422	ASP	2.2
1	A	1376	PRO	2.2
1	A	1732	ALA	2.2
1	B	986	ALA	2.2
1	D	675	GLY	2.2
1	A	1543	ILE	2.2
1	D	677	THR	2.2
1	A	1449	GLU	2.2
1	B	65	ASN	2.2
1	D	1604	THR	2.2
1	B	3	SER	2.2
1	A	632	ARG	2.2
1	C	1001	GLU	2.2
1	C	1376	PRO	2.2
1	A	79	LYS	2.2
1	C	1157	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1117	ASN	2.2
1	C	1413	TYR	2.2
1	B	469	VAL	2.2
1	D	1371	THR	2.2
1	C	1334	ASP	2.2
1	C	1187	GLY	2.1
1	D	541	GLY	2.1
1	B	1225	PRO	2.1
1	B	1551	PRO	2.1
1	A	653	VAL	2.1
1	B	728	SER	2.1
1	D	1184	SER	2.1
1	D	1370	ASP	2.1
1	D	198	SER	2.1
1	A	172	THR	2.1
1	B	6	GLY	2.1
1	C	135	SER	2.1
1	B	566	PRO	2.1
1	B	1272	LYS	2.1
1	A	730	ASP	2.1
1	A	1103	ASP	2.1
1	B	1011	VAL	2.1
1	D	174	THR	2.1
1	C	92	ALA	2.1
1	D	726	GLY	2.1
1	A	739	HIS	2.1
1	C	216	ALA	2.1
1	C	1245	SER	2.1
1	C	1660	PRO	2.1
1	B	494	LYS	2.1
1	C	750	VAL	2.1
1	B	1002	TYR	2.1
1	B	1445	TYR	2.1
1	C	600	ILE	2.1
1	C	893	GLY	2.1
1	C	1357	GLU	2.1
1	C	128	THR	2.1
1	D	93	CYS	2.1
1	A	176	GLY	2.1
1	D	178	GLY	2.1
1	D	573	SER	2.1
1	C	599	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	972	PRO	2.1
1	C	1551	PRO	2.1
1	D	1623	MET	2.1
1	B	1103	ASP	2.1
1	A	1315	HIS	2.1
1	D	468	THR	2.1
1	A	434	LYS	2.1
1	D	1551	PRO	2.1
1	C	1659	HIS	2.1
1	D	1642	ARG	2.1
1	A	1412	LYS	2.1
1	B	1262	CYS	2.1
1	D	908	PHE	2.1
1	A	308	ALA	2.1
1	C	242	GLU	2.1
1	D	1624	TYR	2.1
1	B	745	ALA	2.1
1	D	142	CYS	2.1
1	D	1011	VAL	2.1
1	C	403	ASN	2.1
1	B	1538	ARG	2.0
1	D	232	PRO	2.0
1	C	573	SER	2.0
1	C	606	PHE	2.0
1	D	1053	GLU	2.0
1	D	1143	SER	2.0
1	D	1625	MET	2.0
1	B	955	ALA	2.0
1	A	708	SER	2.0
1	A	296	PRO	2.0
1	B	152	GLY	2.0
1	D	1144	GLY	2.0
1	B	1676	GLU	2.0
1	A	675	GLY	2.0
1	C	303	CYS	2.0
1	A	606	PHE	2.0
1	A	1549	TRP	2.0
1	D	143	VAL	2.0
1	C	1638	GLN	2.0
1	D	584	SER	2.0
1	B	953	SER	2.0
1	D	125	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1312	ALA	2.0
1	D	77	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.