



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2016 – 09:52 AM EDT

PDB ID : 5I6I
Title : Crystal structure of a dBCCP-variant of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on : 2016-02-16
Resolution : 8.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027257

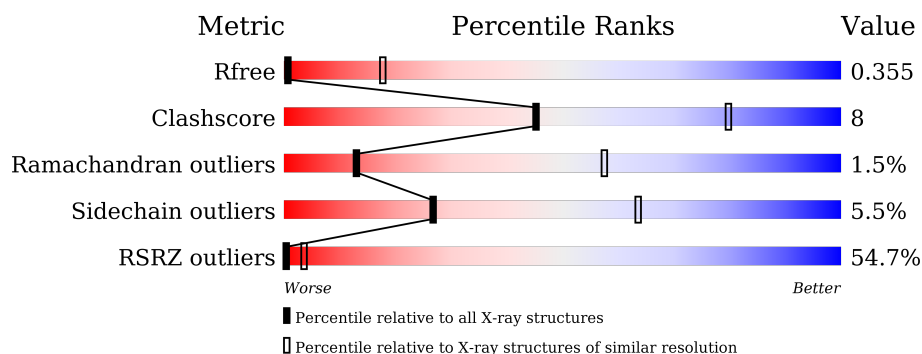
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.40 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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2211	<div> <div>36%</div> <div>48%</div> <div>13%</div> <div>•</div> <div>37%</div> </div>
1	B	2211	<div> <div>33%</div> <div>49%</div> <div>13%</div> <div>•</div> <div>37%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22445 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.

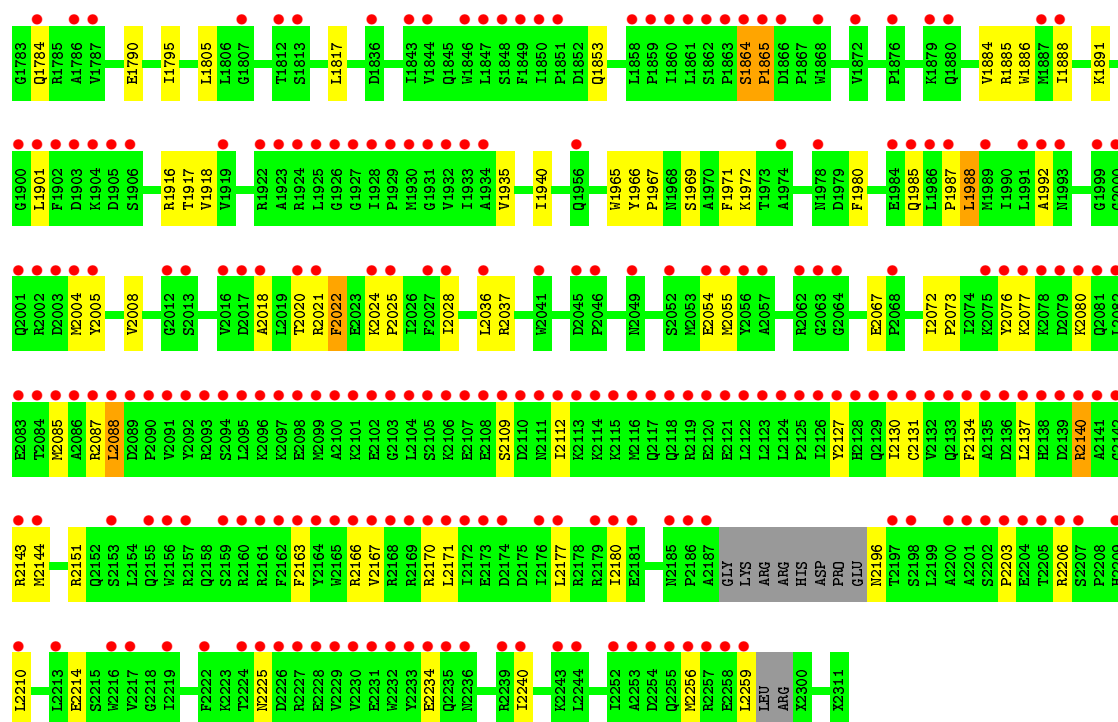
- Molecule 1 is a protein called Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1399	Total	C	N	O	S	0	0	0
			11224	7122	1978	2086	38			
1	B	1394	Total	C	N	O	S	0	0	0
			11221	7120	1976	2086	39			

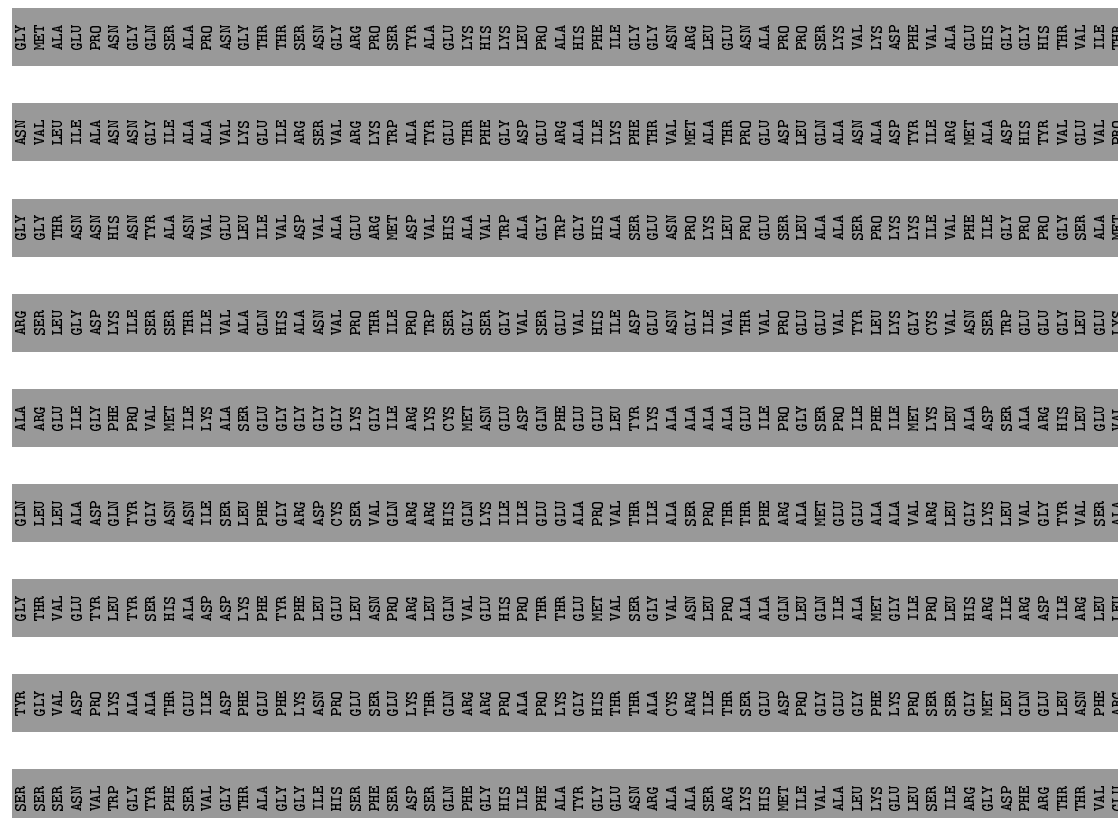
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP G0S3L5
A	763	GLY	-	linker	UNP G0S3L5
A	764	SER	-	linker	UNP G0S3L5
A	765	GLY	-	linker	UNP G0S3L5
B	63	GLY	-	expression tag	UNP G0S3L5
B	763	GLY	-	linker	UNP G0S3L5
B	764	SER	-	linker	UNP G0S3L5
B	765	GLY	-	linker	UNP G0S3L5

D1705	P1619	V1521	E1431	H1351	R1289	LYS	E1162	Y1096	A1025	V965	L904	Q843	LEU
E1706	E1620	S1522	V1432	I1352	V1290	GLN	R1163	Y1097	R1026	V966	E905	Q844	PRO
A1707	V1621	T1523	A1433	I1353	R1291	GLN	D1164	A1098	E1027	V967	P906	P845	GLN
K1708	P1622	P1524	V1354	V1354	R1292	PRO	F1165	L1099	L1028	T968	L907	S846	TTR
R1709	R1625	Y1525	R1451	V1355	L1293	GLY	K1166	A1100	A1100	V969	T908	A847	GLY
R1710	K1626	Y1526	V1452	E1356	T1294	ILE	R1167	A1101	T1030	L970	S909	L848	S788
F1711	F1627	T1527	H1453	R1360	F1295	ALA	I1168	L1102	L1031	S971	V910	H849	P789
E1714	V1629	K1528	Q1454	I1361	L1296	ALA	H1169	E1103	CYS	R972	L911	A850	V790
V1715	V1630	R1529	I1459	G1361	C1297	ASP	S1170	V1104	ALA	R973	N912	R851	V791
I1716	G1542	G1543	N1460	E1362	R1298	LEU	Y1105	V1105	LEU	R974	L913	M852	V792
T1717	T1543	Q1544	G1461	T1364	G1299	ALA	S1171	V1106	PRO	V975	Y914	P853	V793
E1718	A1631	Q1545	K1462	T1364	R1299	GLN	S1172	R1107	SER	R976	L915	H854	G794
E1719	D1633	Y1546	R1463	D1365	G1302	ARG	M1174	R1108	LEU	S977	D916	K855	K795
V1720	I1634	V1546	ASP	Y1368	S1303	ARG	T1175	A1109	GLU	K978	G917	L856	P796
V1721	F1635	F1549	ASN	Y1369	Y1304	ARG	Y1176	Y1110	GLU	R979	Q918	D857	Q797
D1723	P1636	P1550	ASN	F1369	P1305	PRO	L1177	Y1111	GLU	S980	K919	A858	Q798
G1724	K1637	F1551	ASP	R1370	S1306	GLY	A1178	Y1114	T1041	L981	R921	Q859	R799
E1725	I1638	E1551	ASP	A1372	T1307	THR	R1179	N1114	Y1042	V982	R922	L860	F900
K1726	R1657	L1552	E1469	V1373	Y1308	PRO	R1180	L1115	H1044	L983	E923	T861	A801
R1727	K1658	F1553	E1470	V1374	T1309	LEU	T1181	L1116	Y1047	L985	L923	Q862	V802
H1728	P1662	I1557	E1471	R1375	F1310	ARG	D1182	E1117	L1048	L986	L924	V863	L803
K1729	P1663	Q1558	T1472	P1376	R1311	LEU	E1183	Y1120	L1048	L987	L925	L864	Y804
I1730	R1664	S1559	P1473	G1377	P1313	GLY	P1185	R1125	Y1052	E988	A927	R866	T806
I1731	Y1665	S1560	P1474	R1378	D1314	ILE	I1186	P1156	V1053	R989	D928	A867	N807
T1732	Y1666	G1561	ASP	ARG	Y1315	GLY	R1187	F1127	Q1054	R990	L929	Q868	C808
L1733	Y1667	T1562	GLU	GLU	Y1316	LEU	E1188	Y1128	S1055	P991	L930	R869	D809
V1734	E1563	E1563	ILE	ILE	D1319	SER	V1190	I1129	R1056	R992	M932	Q871	L811
G1735	A1564	A1564	T1482	SER	S1320	SER	I1191	D1132	Y1057	P994	Y933	A872	N812
L1674	G1675	T1568	G1483	THR	I1321	V1254	P1192	F1133	G1058	V995	D935	E873	G813
L1676	L1677	I1568	G1484	A1386	I1322	V1255	P1193	ALA	E1059	V996	V936	F874	Y814
L1677	E1677	L1569	F1485	L1389	H1323	V1257	C1194	ALA	W1062	V999	E937	A876	N816
E1678	E1679	A1572	V1486	L1389	I1324	A1258	D1196	ARG	R1066	G1000	Q938	Q877	Q817
V1742	M1681	K1573	I1489	E1392	E1325	R1259	L1197	LYS	P1067	K1001	Q939	Q878	V818
C1744	P1682	Q1575	L1491	E1392	P1326	D1260	L1198	SER	D1068	H1002	F940	L879	V819
L1745	H1683	P1576	L1492	A1403	S1327	D1261	D1199	GLY	D1069	H1003	S941	L880	M820
E1684	F1684	E1493	E1493	A1404	L1328	A1262	ASN	ALA	E1070	L1004	G942	R881	Q821
N1685	N1685	E1405	E1405	E1405	F1330	G1264	GLN	THR	V1071	P1005	R944	V882	Q822
A1687	A1687	I1406	I1406	I1406	F1330	K1265	L1204	THR	E1074	L1006	L945	F883	K823
H1688	H1688	G1408	G1408	G1408	E1333	N1266	L1204	GLU	E1074	L1007	Q946	K884	L824
N1689	N1689	T1409	T1409	T1409	L1334	D1267	S1205	SER	V1075	R1008	D947	K885	K825
V1503	V1503	N1410	N1410	N1410	G1335	E1268	A1207	SER	V1075	R1009	E948	F886	E826
Y1504	Y1504	M1415	M1415	M1415	R1336	E1269	L1208	MET	S1078	L1010	E949	L887	F827
Y1505	Y1505	H1416	H1416	H1416	L1337	I1270	HIS	GLN	T1078	T1011	A950	D888	E828
V1507	V1507	M1417	M1417	M1417	S1338	L1271	MET	GLN	Y1080	E1012	I951	D889	E829
S1508	S1508	F1418	F1418	F1418	F1340	L1271	L1211	SER	V1082	E1014	L952	N890	V830
A1511	A1511	H1423	H1423	H1423	K1341	K1275	ALA	VAL	F1083	S1015	L954	P892	L831
K1512	K1512	T1424	T1424	T1424	P1344	V1277	LYS	S1153	V1085	R894	D956	H893	D832
M1516	M1516	Q1426	Q1426	Q1426	P1345	V1278	GLU	S1155	D1084	S1016	Q1017	K895	D833
H1517	H1517	V1427	V1427	V1427	F1346	THR	THR	P1087	V1087	Q1017	D956	T895	P834
L1701	L1701	T1428	T1428	T1428	T1347	L1285	LYS	A1158	F1089	S1018	K959	D898	P837
Y1702	Y1702	L1429	L1429	L1429	Q1349	L1286	ASP	A1159	F1090	A1019	D960	L899	P837
L1703	L1703	D1430	D1430	D1430	K1350	L1287	LYS	T1159	F1091	K1020	L899	L900	S839
S1704	S1704	D1430	D1430	D1430	K1350	L1288	ARG	V1161	A1091	V1021	N861	L900	S839
										S1022	P862	L900	S839
										L1023	Q963	F841	F841
										K1024	K964	T903	S842



- Molecule 1: Acetyl-CoA carboxylase-like protein, Acetyl-CoA carboxylase-like protein, Acetyl-CoA carboxylase-like protein







4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	462.20 Å 462.20 Å 204.64 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.95 – 8.40 49.95 – 8.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.95-8.40) 99.8 (49.95-8.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 8.33 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.297 , 0.324 0.322 , 0.355	Depositor DCC
R_{free} test set	548 reflections (4.53%)	DCC
Wilson B-factor (Å ²)	572.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 897.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	22445	wwPDB-VP
Average B, all atoms (Å ²)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/11401	0.64	0/15435
1	B	0.41	0/11458	0.63	0/15511
All	All	0.41	0/22859	0.63	0/30946

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11224	0	11148	178	0
1	B	11221	0	11191	174	0
All	All	22445	0	22339	347	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 8.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:VAL:HG21	1:A:1203:ALA:HB1	1.48	0.94
1:B:1108:ARG:HH21	1:B:1375:ARG:HH22	1.21	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.65	0.79
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.65	0.79
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.65	0.78
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.69	0.75
1:B:1091:ALA:HB2	1:B:1260:ARG:HG2	1.66	0.75
1:B:1131:TRP:O	1:B:1188:LYS:HA	1.87	0.74
1:B:1462:MET:HG2	1:B:1470:ASN:HB2	1.69	0.74
1:B:1415:ASN:HB2	1:B:1452:VAL:HA	1.71	0.73
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.72	0.72
1:B:1516:MET:HG3	1:B:1519:LEU:HD12	1.71	0.71
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.71	0.70
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.71	0.70
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.75	0.68
1:A:961:ASN:HA	1:A:964:LYS:HB2	1.74	0.68
1:B:961:ASN:HA	1:B:964:LYS:HB2	1.74	0.68
1:A:1007:LEU:HD12	1:A:1029:LEU:HG	1.76	0.67
1:B:1007:LEU:HD12	1:B:1029:LEU:HG	1.77	0.67
1:B:2037:ARG:HE	1:B:2067:GLU:HA	1.59	0.67
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.75	0.67
1:B:926:ILE:HD12	1:B:985:LEU:HD11	1.78	0.66
1:B:1376:PRO:HB3	1:B:1423:HIS:HB2	1.77	0.66
1:B:1127:TYR:HB2	1:B:1193:PRO:HD2	1.78	0.65
1:B:1299:ARG:HD2	1:B:1303:SER:HB2	1.78	0.65
1:B:1180:ARG:HD2	1:B:1182:ARG:HD3	1.79	0.64
1:A:926:ILE:HD12	1:A:985:LEU:HD11	1.78	0.64
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.80	0.63
1:A:1171:ILE:HG23	1:A:1330:PHE:HB2	1.80	0.63
1:A:1180:ARG:HD2	1:A:1182:ARG:HD3	1.79	0.63
1:A:1195:LYS:HA	1:A:1260:ARG:HD2	1.81	0.63
1:A:848:LEU:HD23	1:A:851:ARG:HG3	1.81	0.63
1:B:1427:VAL:HG11	1:B:1459:ILE:HD12	1.80	0.63
1:A:1087:THR:HG21	1:A:1305:PRO:HG2	1.80	0.62
1:B:1007:LEU:HD11	1:B:1025:ALA:O	2.00	0.62
1:B:848:LEU:HD23	1:B:851:ARG:HG3	1.81	0.62
1:A:1007:LEU:HD11	1:A:1025:ALA:O	2.00	0.62
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.82	0.61
1:A:880:LEU:HD13	1:A:915:LEU:HD13	1.80	0.61
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.82	0.61
1:A:1161:VAL:HB	1:A:1330:PHE:HZ	1.66	0.60
1:B:1176:TYR:CE2	1:B:1291:ARG:HD3	2.36	0.60
1:A:1168:ILE:HB	1:A:1181:THR:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.83	0.60
1:A:1376:PRO:HG2	1:A:1423:HIS:HB2	1.82	0.60
1:B:1108:ARG:HH21	1:B:1375:ARG:NH2	1.96	0.60
1:A:1517:HIS:HB3	1:A:1598:VAL:HG23	1.84	0.60
1:A:852:MET:HB3	1:A:853:PRO:HD2	1.83	0.60
1:B:1341:LYS:HG3	1:B:1360:ARG:HG2	1.84	0.60
1:B:852:MET:HB3	1:B:853:PRO:HD2	1.83	0.60
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.85	0.59
1:A:1091:ALA:CB	1:A:1260:ARG:HG2	2.33	0.59
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.66	0.59
1:B:1090:PHE:HB2	1:B:1193:PRO:HB3	1.85	0.59
1:A:2163:PHE:O	1:A:2167:VAL:HG23	2.03	0.59
1:B:1116:ARG:HE	1:B:1132:ASP:HB2	1.66	0.58
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.85	0.58
1:B:2163:PHE:O	1:B:2167:VAL:HG23	2.04	0.58
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.86	0.58
1:B:1549:PHE:O	1:B:1553:PHE:HD1	1.87	0.58
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.85	0.58
1:A:1304:TYR:HB3	1:A:1350:LYS:HB2	1.86	0.58
1:B:1156:SER:HB2	1:B:1157:PRO:HD3	1.85	0.58
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.86	0.58
1:A:1068:ASP:HB3	1:A:1071:VAL:HG23	1.86	0.57
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.70	0.57
1:B:887:LEU:HD22	1:B:900:LEU:HB3	1.86	0.57
1:A:1162:GLU:HG3	1:A:1501:GLU:HG2	1.86	0.57
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.87	0.57
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.86	0.57
1:A:1087:THR:CB	1:A:1298:GLY:HA3	2.34	0.57
1:A:1549:PHE:O	1:A:1553:PHE:HD1	1.86	0.57
1:B:1884:VAL:HG21	1:B:1935:VAL:O	2.04	0.57
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.87	0.57
1:B:1081:THR:HG23	1:B:1375:ARG:HE	1.70	0.57
1:B:1517:HIS:HB3	1:B:1598:VAL:HG23	1.86	0.57
1:A:1884:VAL:HG21	1:A:1935:VAL:O	2.04	0.57
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.86	0.56
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.87	0.56
1:B:1059:GLU:HB3	1:B:1062:TRP:HZ3	1.70	0.56
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.86	0.56
1:A:1307:TYR:H	1:A:1323:HIS:HA	1.71	0.56
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.86	0.56
1:A:1087:THR:HG21	1:A:1305:PRO:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:LEU:HD22	1:A:900:LEU:HB3	1.87	0.56
1:B:1068:ASP:HB3	1:B:1071:VAL:HG23	1.88	0.56
1:A:1059:GLU:HB3	1:A:1062:TRP:HZ3	1.71	0.55
1:A:1156:SER:HB2	1:A:1157:PRO:HD3	1.87	0.55
1:A:1087:THR:OG1	1:A:1298:GLY:HA3	2.05	0.55
1:A:2072:ILE:HD12	1:A:2131:CYS:HB2	1.89	0.55
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.06	0.55
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.89	0.55
1:A:936:VAL:HG23	1:A:968:THR:HG23	1.89	0.55
1:B:1492:TYR:HA	1:B:1506:TYR:HA	1.87	0.55
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.88	0.55
1:B:936:VAL:HG23	1:B:968:THR:HG23	1.88	0.54
1:B:2072:ILE:HD12	1:B:2131:CYS:HB2	1.89	0.54
1:A:1333:GLU:HG2	1:A:1336:ARG:HG3	1.90	0.54
1:B:1516:MET:H	1:B:1600:ARG:HA	1.73	0.54
1:B:1176:TYR:HE2	1:B:1291:ARG:HD3	1.72	0.53
1:A:1371:ARG:HD3	1:A:1418:PHE:HB3	1.90	0.53
1:A:1295:PHE:O	1:A:1307:TYR:HA	2.07	0.53
1:A:1087:THR:HB	1:A:1298:GLY:HA3	1.91	0.53
1:B:1132:ASP:HA	1:B:1187:ARG:O	2.08	0.53
1:A:2037:ARG:HE	1:A:2067:GLU:HA	1.74	0.52
1:B:1116:ARG:HE	1:B:1132:ASP:CB	2.23	0.52
1:B:922:GLU:O	1:B:926:ILE:HG12	2.09	0.52
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.92	0.52
1:A:2256:MET:HA	1:A:2259:LEU:HD12	1.92	0.52
1:A:922:GLU:O	1:A:926:ILE:HG12	2.10	0.52
1:B:1059:GLU:HB3	1:B:1062:TRP:CZ3	2.45	0.52
1:B:1985:GLN:HB3	1:B:2024:LYS:HE3	1.92	0.52
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.92	0.51
1:A:1008:ARG:O	1:A:1011:THR:HG22	2.10	0.51
1:B:1133:PHE:HB2	1:B:1187:ARG:HB2	1.92	0.51
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.92	0.51
1:A:1702:TYR:HA	1:A:1729:LYS:HA	1.92	0.51
1:B:1702:TYR:HA	1:B:1729:LYS:HA	1.93	0.51
1:B:1026:ARG:HG2	1:B:1391:SER:OG	2.11	0.51
1:A:1333:GLU:CG	1:A:1336:ARG:HG3	2.41	0.51
1:A:1054:GLN:HB3	1:A:1062:TRP:CD1	2.46	0.51
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	1.92	0.51
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.92	0.51
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.93	0.51
1:B:1006:VAL:O	1:B:1009:ARG:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:ARG:O	1:B:1011:THR:HG22	2.10	0.50
1:B:1506:TYR:H	1:B:1517:HIS:CE1	2.30	0.50
1:A:1340:PHE:CZ	1:A:1527:THR:HG22	2.47	0.50
1:B:1054:GLN:HB3	1:B:1062:TRP:CD1	2.47	0.50
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.93	0.50
1:A:1492:TYR:CD1	1:A:1506:TYR:HB3	2.46	0.50
1:B:1091:ALA:HB2	1:B:1260:ARG:CG	2.39	0.50
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.93	0.50
1:A:1006:VAL:O	1:A:1009:ARG:HG2	2.11	0.50
1:A:907:LEU:O	1:A:911:LEU:HD13	2.12	0.50
1:A:1059:GLU:HB3	1:A:1062:TRP:CZ3	2.46	0.50
1:A:1091:ALA:HB1	1:A:1260:ARG:HG2	1.94	0.50
1:A:856:LEU:HB2	1:A:894:LYS:HE2	1.94	0.50
1:B:2210:LEU:O	1:B:2214:GLU:HB2	2.12	0.49
1:B:1535:ARG:HA	1:B:1545:TYR:HB2	1.94	0.49
1:A:1120:TYR:HD1	1:A:1129:ILE:HG22	1.78	0.49
1:A:1154:PRO:HB2	1:A:1158:ALA:HB2	1.93	0.49
1:B:907:LEU:O	1:B:911:LEU:HD13	2.12	0.49
1:A:1516:MET:H	1:A:1600:ARG:HA	1.77	0.49
1:A:1985:GLN:HB3	1:A:2024:LYS:HE3	1.93	0.49
1:B:1265:LYS:HE3	1:B:1299:ARG:HG3	1.93	0.49
1:B:1429:ALA:HB2	1:B:1475:LEU:HD13	1.94	0.49
1:A:827:PHE:O	1:A:831:LEU:HD23	2.13	0.49
1:B:1168:ILE:HB	1:B:1181:THR:HG21	1.95	0.49
1:A:1099:LEU:HA	1:A:1102:LEU:HD12	1.95	0.49
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.77	0.49
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.94	0.49
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.78	0.49
1:B:827:PHE:O	1:B:831:LEU:HD23	2.13	0.49
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.78	0.48
1:A:1328:LEU:HD22	1:A:1373:VAL:HG21	1.94	0.48
1:A:1980:PHE:CB	1:A:1988:LEU:HD21	2.43	0.48
1:A:2028:ILE:HB	1:A:2055:MET:HG3	1.94	0.48
1:A:2210:LEU:O	1:A:2214:GLU:HB2	2.12	0.48
1:A:860:LEU:HG	1:A:879:LEU:HD22	1.95	0.48
1:B:860:LEU:HG	1:B:879:LEU:HD22	1.95	0.48
1:B:1053:VAL:HG23	1:B:1062:TRP:HB3	1.95	0.48
1:A:1091:ALA:HB2	1:A:1260:ARG:HG2	1.94	0.48
1:B:1192:VAL:HG11	1:B:1203:ALA:O	2.13	0.48
1:B:2028:ILE:HB	1:B:2055:MET:HG3	1.94	0.48
1:B:856:LEU:HB2	1:B:894:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:VAL:HG23	1:A:1062:TRP:HB3	1.96	0.47
1:A:1293:LEU:O	1:A:1309:THR:HA	2.15	0.47
1:B:895:THR:O	1:B:895:THR:HG23	2.15	0.47
1:B:895:THR:HB	1:B:900:LEU:HD12	1.95	0.47
1:A:895:THR:HB	1:A:900:LEU:HD12	1.95	0.47
1:A:1174:MET:SD	1:A:1335:GLY:HA3	2.55	0.47
1:A:1516:MET:HG3	1:A:1519:LEU:HD22	1.96	0.47
1:A:1056:ARG:HD2	1:A:1062:TRP:CZ2	2.50	0.47
1:A:1090:PHE:HB2	1:A:1193:PRO:HB3	1.97	0.47
1:B:1403:ALA:O	1:B:1406:ILE:HG13	2.15	0.47
1:A:1426:GLN:HG3	1:A:1462:MET:HB3	1.97	0.47
1:B:1966:TYR:H	1:B:1969:SER:HB2	1.80	0.47
1:A:895:THR:O	1:A:895:THR:HG23	2.15	0.47
1:A:1403:ALA:O	1:A:1406:ILE:HG13	2.14	0.46
1:A:1886:TRP:HB3	1:A:1891:LYS:HB2	1.98	0.46
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.97	0.46
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.97	0.46
1:A:1266:ASN:HB2	1:A:1270:ILE:HB	1.97	0.46
1:B:1056:ARG:HD2	1:B:1062:TRP:CZ2	2.50	0.46
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	1.98	0.46
1:A:1102:LEU:O	1:A:1106:VAL:HG23	2.15	0.46
1:B:1155:SER:HB2	1:B:1168:ILE:HG12	1.98	0.46
1:A:1492:TYR:CD1	1:A:1504:TYR:HB3	2.50	0.46
1:A:1966:TYR:H	1:A:1969:SER:HB2	1.81	0.46
1:A:894:LYS:HG3	1:A:900:LEU:CD1	2.46	0.46
1:B:1096:TYR:CD1	1:B:1096:TYR:C	2.89	0.46
1:B:1102:LEU:HD21	1:B:1193:PRO:HG3	1.97	0.46
1:B:1127:TYR:OH	1:B:1207:ALA:HB1	2.16	0.46
1:A:1416:HIS:HD2	1:A:1454:GLN:HG3	1.80	0.46
1:B:2203:PRO:HA	1:B:2206:ARG:HB3	1.97	0.46
1:B:2037:ARG:HH11	1:B:2068:PRO:HD3	1.81	0.46
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.98	0.46
1:B:945:LEU:HD13	1:B:951:ILE:HG13	1.98	0.46
1:A:1155:SER:HB2	1:A:1168:ILE:HG12	1.98	0.46
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	1.98	0.46
1:B:1531:LEU:HG	1:B:1535:ARG:HD2	1.98	0.46
1:B:1154:PRO:HB2	1:B:1158:ALA:HB2	1.97	0.45
1:B:933:TYR:HD1	1:B:978:LYS:HG2	1.81	0.45
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	1.98	0.45
1:B:1531:LEU:HD23	1:B:1535:ARG:NH1	2.31	0.45
1:A:1255:VAL:O	1:A:1293:LEU:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:LEU:HD11	1:A:1600:ARG:HD2	1.97	0.45
1:A:1096:TYR:C	1:A:1096:TYR:CD1	2.89	0.45
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.99	0.45
1:B:1253:ALA:O	1:B:1291:ARG:HG2	2.16	0.45
1:A:904:LEU:O	1:A:908:THR:HG23	2.17	0.45
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.98	0.45
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.99	0.45
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.99	0.45
1:B:1323:HIS:CE1	1:B:1350:LYS:HD2	2.51	0.45
1:A:2020:THR:HG21	1:B:1757:ARG:HG2	1.98	0.45
1:A:887:LEU:HD21	1:A:904:LEU:HD12	1.99	0.45
1:B:1268:GLU:HA	1:B:1271:LEU:HD12	1.97	0.45
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.99	0.45
1:B:894:LYS:HG3	1:B:900:LEU:CD1	2.46	0.45
1:B:810:ILE:HD13	1:B:981:LEU:HD21	1.98	0.45
1:A:810:ILE:HD13	1:A:981:LEU:HD21	1.98	0.45
1:B:1291:ARG:HG3	1:B:1292:ARG:N	2.32	0.45
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	2.00	0.44
1:A:846:SER:HA	1:A:849:HIS:ND1	2.32	0.44
1:A:2144:MET:HG2	1:B:1742:VAL:HG11	1.98	0.44
1:A:1087:THR:HG22	1:A:1296:ILE:HD11	1.99	0.44
1:B:1864:SER:HB2	1:B:1865:PRO:CD	2.43	0.44
1:A:1127:TYR:OH	1:A:1207:ALA:HB1	2.17	0.44
1:A:1689:ASN:HA	1:A:1699:LYS:HE3	2.00	0.44
1:A:923:LEU:HD21	1:A:999:VAL:HG12	2.00	0.44
1:A:1629:VAL:HG22	1:A:1664:ILE:HB	1.99	0.44
1:A:933:TYR:HD1	1:A:978:LYS:HG2	1.82	0.44
1:B:846:SER:HA	1:B:849:HIS:ND1	2.33	0.44
1:A:1378:ARG:HD3	1:A:1392:GLU:HG2	1.99	0.44
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.58	0.44
1:B:1192:VAL:CG1	1:B:1203:ALA:HB1	2.48	0.44
1:A:887:LEU:HD11	1:A:904:LEU:HB2	2.00	0.44
1:B:1153:VAL:N	1:B:1154:PRO:CD	2.81	0.44
1:B:824:LEU:O	1:B:828:ILE:HG12	2.18	0.44
1:A:1052:VAL:HG22	1:A:1096:TYR:CE1	2.53	0.44
1:A:824:LEU:O	1:A:828:ILE:HG12	2.18	0.44
1:B:2109:SER:HA	1:B:2112:ILE:HD12	2.00	0.44
1:B:1087:THR:OG1	1:B:1298:GLY:HA3	2.17	0.44
1:A:1757:ARG:HG2	1:B:2020:THR:HG21	2.00	0.43
1:A:2109:SER:HA	1:A:2112:ILE:HD12	1.99	0.43
1:B:1544:GLN:HG3	1:B:1552:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1742:VAL:HA	1:B:1745:LEU:HD12	1.99	0.43
1:B:904:LEU:O	1:B:908:THR:HG23	2.18	0.43
1:A:1096:TYR:O	1:A:1099:LEU:HB3	2.18	0.43
1:A:945:LEU:HD13	1:A:951:ILE:HG13	2.00	0.43
1:B:891:VAL:HA	1:B:895:THR:HG22	2.01	0.43
1:A:1048:LEU:O	1:A:1052:VAL:HG23	2.18	0.43
1:A:891:VAL:HA	1:A:895:THR:HG22	2.00	0.43
1:B:1116:ARG:NE	1:B:1132:ASP:HB2	2.31	0.43
1:B:1081:THR:OG1	1:B:1375:ARG:HB3	2.19	0.43
1:B:1689:ASN:HA	1:B:1699:LYS:HE3	1.99	0.43
1:B:887:LEU:HD21	1:B:904:LEU:HD12	1.99	0.43
1:A:1258:ALA:HA	1:A:1296:ILE:HG23	2.00	0.43
1:A:2177:LEU:HA	1:A:2180:ILE:HD12	2.00	0.43
1:A:856:LEU:CB	1:A:894:LYS:HE2	2.48	0.43
1:B:975:VAL:HG11	1:B:1017:GLN:HG2	2.01	0.43
1:B:1052:VAL:HG22	1:B:1096:TYR:CE1	2.54	0.43
1:B:1739:GLY:HA2	1:B:1744:CYS:SG	2.58	0.43
1:A:1266:ASN:CB	1:A:1270:ILE:HB	2.49	0.43
1:A:1262:ALA:HB2	1:A:1298:GLY:O	2.19	0.43
1:B:831:LEU:HD12	1:B:922:GLU:HA	2.01	0.43
1:A:1066:ARG:HH12	1:A:1120:TYR:HB3	1.84	0.43
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.22	0.43
1:A:1742:VAL:HA	1:A:1745:LEU:HD12	1.99	0.43
1:B:1164:ASP:H	1:B:1167:ARG:NE	2.17	0.43
1:B:1108:ARG:NH2	1:B:1375:ARG:HH22	2.03	0.43
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	2.01	0.43
1:A:1164:ASP:H	1:A:1167:ARG:NE	2.17	0.43
1:B:1099:LEU:HA	1:B:1102:LEU:HD12	2.00	0.43
1:A:831:LEU:HD12	1:A:922:GLU:HA	2.01	0.42
1:B:1096:TYR:O	1:B:1099:LEU:HB3	2.19	0.42
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.83	0.42
1:B:1629:VAL:HG22	1:B:1664:ILE:HB	2.00	0.42
1:A:2137:LEU:HA	1:A:2140:ARG:HD3	2.00	0.42
1:A:1631:ALA:HB2	1:A:1666:LEU:HB2	2.01	0.42
1:A:2085:MET:C	1:A:2087:ARG:H	2.23	0.42
1:A:831:LEU:HD13	1:A:921:ARG:CZ	2.49	0.42
1:A:836:LEU:HG	1:A:921:ARG:HH12	1.84	0.42
1:A:1040:ARG:HH21	1:A:1085:VAL:HB	1.84	0.42
1:A:1389:LEU:HD11	1:A:1425:PHE:CG	2.53	0.42
1:B:1275:LYS:N	1:B:1276:PRO:HD2	2.34	0.42
1:B:856:LEU:CB	1:B:894:LYS:HE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:LEU:HD13	1:B:921:ARG:CZ	2.49	0.42
1:A:1325:GLU:HG3	1:A:1327:SER:H	1.83	0.42
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.22	0.42
1:B:2085:MET:C	1:B:2087:ARG:H	2.23	0.42
1:A:1275:LYS:N	1:A:1276:PRO:HD2	2.35	0.42
1:A:1291:ARG:HE	1:A:1291:ARG:HB2	1.73	0.42
1:A:975:VAL:HG11	1:A:1017:GLN:HG2	2.02	0.42
1:A:1259:VAL:HG23	1:A:1297:CYS:HA	2.02	0.41
1:B:1170:SER:HB2	1:B:1187:ARG:HH22	1.85	0.41
1:B:1170:SER:HB3	1:B:1173:ASP:HB3	2.02	0.41
1:B:1631:ALA:HB2	1:B:1666:LEU:HB2	2.02	0.41
1:B:887:LEU:HD11	1:B:904:LEU:HB2	2.01	0.41
1:B:1048:LEU:O	1:B:1052:VAL:HG23	2.19	0.41
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.20	0.41
1:A:2018:ALA:HA	1:A:2021:ARG:HD2	2.01	0.41
1:A:1052:VAL:HG22	1:A:1096:TYR:CD1	2.56	0.41
1:A:1504:TYR:HE1	1:A:1521:VAL:HA	1.86	0.41
1:A:2203:PRO:HA	1:A:2206:ARG:HB3	2.01	0.41
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.21	0.41
1:B:1052:VAL:HG22	1:B:1096:TYR:CD1	2.56	0.41
1:B:1504:TYR:CE1	1:B:1521:VAL:HA	2.56	0.41
1:A:1275:LYS:HA	1:A:1278:VAL:HG12	2.03	0.41
1:A:1208:LEU:HD21	1:A:1285:LEU:HD23	2.03	0.41
1:A:961:ASN:O	1:A:965:VAL:HG23	2.21	0.41
1:B:836:LEU:HG	1:B:921:ARG:HH12	1.84	0.41
1:A:1544:GLN:HG3	1:A:1552:LEU:HD11	2.02	0.41
1:B:1098:ALA:O	1:B:1102:LEU:HG	2.21	0.41
1:B:1127:TYR:CG	1:B:1128:PHE:N	2.88	0.41
1:B:1265:LYS:HG3	1:B:1299:ARG:HE	1.86	0.41
1:B:820:MET:HA	1:B:823:LYS:HE3	2.03	0.41
1:A:2088:LEU:HG	1:B:1686:VAL:HG23	2.01	0.41
1:B:1027:GLU:O	1:B:1031:LEU:HG	2.20	0.41
1:B:1066:ARG:HH12	1:B:1120:TYR:HB3	1.86	0.41
1:B:1319:ASP:C	1:B:1344:PRO:HG2	2.41	0.41
1:A:1460:ASN:HD22	1:A:1472:THR:HG21	1.86	0.41
1:A:1524:PRO:O	1:A:1525:TYR:C	2.60	0.41
1:B:1054:GLN:HB3	1:B:1062:TRP:NE1	2.36	0.41
1:A:1054:GLN:HB3	1:A:1062:TRP:NE1	2.36	0.41
1:A:1341:LYS:HG3	1:A:1360:ARG:HG2	2.02	0.41
1:A:2134:PHE:HA	1:A:2137:LEU:HD12	2.03	0.41
1:B:1076:VAL:HG11	1:B:1107:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:LEU:HD21	1:B:999:VAL:HG12	2.01	0.41
1:B:1007:LEU:HD11	1:B:1025:ALA:C	2.41	0.40
1:B:1530:TRP:O	1:B:1533:PRO:HD2	2.21	0.40
1:A:1864:SER:HB2	1:A:1865:PRO:CD	2.43	0.40
1:A:1988:LEU:HG	1:A:2022:PHE:CZ	2.57	0.40
1:A:1987:PRO:HG3	1:A:2171:LEU:HD21	2.03	0.40
1:B:1162:GLU:HG3	1:B:1522:SER:OG	2.20	0.40
1:B:993:LYS:HG2	1:B:1031:LEU:HD22	2.03	0.40
1:B:1794:ILE:HD12	1:B:1823:MET:HG3	2.04	0.40
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.42	0.40
1:B:1340:PHE:CZ	1:B:1527:THR:HG22	2.56	0.40
1:A:2005:TYR:HA	1:B:1826:ASN:HD22	1.87	0.40
1:A:1125:ARG:HH22	1:A:1199:ASP:CG	2.25	0.40
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.87	0.40
1:A:820:MET:HA	1:A:823:LYS:HE3	2.02	0.40
1:B:1052:VAL:HA	1:B:1096:TYR:CZ	2.57	0.40
1:B:1527:THR:O	1:B:1530:TRP:CD1	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1373/2211 (62%)	1229 (90%)	123 (9%)	21 (2%)	13	57
1	B	1380/2211 (62%)	1249 (90%)	110 (8%)	21 (2%)	13	57
All	All	2753/4422 (62%)	2478 (90%)	233 (8%)	42 (2%)	13	57

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	943	ARG

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Mol	Chain	Res	Type
1	A	1156	SER
1	A	1516	MET
1	A	1784	GLN
1	A	1864	SER
1	B	943	ARG
1	B	1092	HIS
1	B	1156	SER
1	B	1864	SER
1	A	887	LEU
1	A	1128	PHE
1	A	1180	ARG
1	A	2225	ASN
1	B	887	LEU
1	B	1180	ARG
1	A	853	PRO
1	A	1486	VAL
1	A	1512	LYS
1	B	853	PRO
1	B	1160	PRO
1	B	1426	GLN
1	B	1516	MET
1	B	1638	ILE
1	B	1784	GLN
1	B	2225	ASN
1	A	892	PRO
1	A	1333	GLU
1	A	1638	ILE
1	A	1790	GLU
1	B	892	PRO
1	B	1128	PHE
1	B	1486	VAL
1	B	1790	GLU
1	A	1313	PRO
1	A	1317	GLU
1	A	1865	PRO
1	B	1313	PRO
1	B	1865	PRO
1	B	1317	GLU
1	A	1052	VAL
1	B	1052	VAL
1	A	1525	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1208/1879 (64%)	1138 (94%)	70 (6%)	25	61
1	B	1215/1879 (65%)	1151 (95%)	64 (5%)	28	64
All	All	2423/3758 (64%)	2289 (94%)	134 (6%)	27	63

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	819	VAL
1	A	836	LEU
1	A	848	LEU
1	A	852	MET
1	A	880	LEU
1	A	883	PHE
1	A	884	ASN
1	A	911	LEU
1	A	913	LEU
1	A	921	ARG
1	A	930	LEU
1	A	951	ILE
1	A	952	LEU
1	A	954	LEU
1	A	961	ASN
1	A	970	LEU
1	A	1007	LEU
1	A	1021	VAL
1	A	1062	TRP
1	A	1079	LYS
1	A	1086	LEU
1	A	1090	PHE
1	A	1096	TYR
1	A	1115	LEU
1	A	1127	TYR
1	A	1132	ASP
1	A	1171	ILE

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Mol	Chain	Res	Type
1	A	1177	LEU
1	A	1259	VAL
1	A	1261	ASP
1	A	1291	ARG
1	A	1320	SER
1	A	1342	LEU
1	A	1343	THR
1	A	1378	ARG
1	A	1379	LEU
1	A	1424	THR
1	A	1462	MET
1	A	1475	LEU
1	A	1489	ILE
1	A	1551	GLU
1	A	1557	ILE
1	A	1563	GLU
1	A	1593	ASP
1	A	1595	LEU
1	A	1618	THR
1	A	1632	ASN
1	A	1638	ILE
1	A	1674	LEU
1	A	1715	VAL
1	A	1771	ARG
1	A	1805	LEU
1	A	1817	LEU
1	A	1853	GLN
1	A	1901	LEU
1	A	1917	THR
1	A	1965	TRP
1	A	1967	PRO
1	A	1971	PHE
1	A	1988	LEU
1	A	2022	PHE
1	A	2076	TYR
1	A	2088	LEU
1	A	2140	ARG
1	A	2143	ARG
1	A	2151	ARG
1	A	2166	ARG
1	A	2196	ASN
1	A	2234	GLU

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Mol	Chain	Res	Type
1	A	2240	ILE
1	B	819	VAL
1	B	836	LEU
1	B	848	LEU
1	B	852	MET
1	B	880	LEU
1	B	883	PHE
1	B	884	ASN
1	B	911	LEU
1	B	913	LEU
1	B	915	LEU
1	B	921	ARG
1	B	930	LEU
1	B	951	ILE
1	B	952	LEU
1	B	954	LEU
1	B	961	ASN
1	B	970	LEU
1	B	1007	LEU
1	B	1021	VAL
1	B	1032	CYS
1	B	1062	TRP
1	B	1086	LEU
1	B	1090	PHE
1	B	1096	TYR
1	B	1115	LEU
1	B	1116	ARG
1	B	1127	TYR
1	B	1177	LEU
1	B	1192	VAL
1	B	1254	VAL
1	B	1296	ILE
1	B	1324	ILE
1	B	1327	SER
1	B	1331	GLN
1	B	1378	ARG
1	B	1430	ASP
1	B	1551	GLU
1	B	1557	ILE
1	B	1563	GLU
1	B	1593	ASP
1	B	1595	LEU

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Mol	Chain	Res	Type
1	B	1618	THR
1	B	1632	ASN
1	B	1638	ILE
1	B	1674	LEU
1	B	1715	VAL
1	B	1771	ARG
1	B	1805	LEU
1	B	1817	LEU
1	B	1845	GLN
1	B	1853	GLN
1	B	1901	LEU
1	B	1917	THR
1	B	1965	TRP
1	B	1967	PRO
1	B	1971	PHE
1	B	2076	TYR
1	B	2088	LEU
1	B	2139	ASP
1	B	2140	ARG
1	B	2143	ARG
1	B	2151	ARG
1	B	2166	ARG
1	B	2196	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1415	ASN

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	1387/2211 (62%)	3.37	787 (56%) 0 3	25, 211, 483, 500	0
1	B	1394/2211 (63%)	3.07	734 (52%) 0 4	5, 245, 486, 500	0
All	All	2781/4422 (62%)	3.22	1521 (54%) 0 3	5, 230, 485, 500	0

All (1521) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	875	PRO	21.0
1	A	1155	SER	18.6
1	B	874	PHE	18.3
1	A	1685	ASN	18.2
1	A	926	ILE	17.4
1	A	2089	ASP	17.2
1	B	879	LEU	17.2
1	A	1169	HIS	16.4
1	B	2131	CYS	15.8
1	B	903	THR	15.7
1	A	841	PHE	15.6
1	A	1686	VAL	15.2
1	B	1685	ASN	15.1
1	B	2123	LEU	15.0
1	B	1256	ASN	14.8
1	A	1253	ALA	14.8
1	B	841	PHE	14.7
1	A	846	SER	14.5
1	B	2216	TRP	14.4
1	B	1701	LEU	14.3
1	A	1694	PRO	14.3
1	B	893	ASN	14.3
1	A	2120	GLU	14.1
1	B	2130	ILE	14.1

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Mol	Chain	Res	Type	RSRZ
1	B	1686	VAL	14.0
1	B	2217	VAL	14.0
1	B	2127	TYR	13.8
1	A	985	LEU	13.8
1	A	845	PHE	13.5
1	A	1688	TRP	13.5
1	B	852	MET	13.5
1	A	1003	LEU	13.3
1	A	838	TYR	13.3
1	A	1687	ALA	13.1
1	B	1190	VAL	13.1
1	A	939	GLN	13.1
1	A	1181	THR	12.7
1	A	837	PRO	12.6
1	A	842	SER	12.4
1	B	853	PRO	12.4
1	A	1184	GLU	12.4
1	A	1163	ASN	12.3
1	B	2229	VAL	12.3
1	A	874	PHE	12.2
1	A	2088	LEU	12.2
1	A	1702	TYR	12.2
1	B	894	LYS	12.1
1	A	1684	PHE	12.1
1	B	1474	PRO	12.1
1	B	2088	LEU	11.7
1	A	2085	MET	11.7
1	B	842	SER	11.7
1	B	1185	PRO	11.6
1	A	849	HIS	11.6
1	A	1168	ILE	11.5
1	A	791	VAL	11.5
1	B	1103	GLU	11.5
1	A	1575	GLN	11.4
1	A	946	GLN	11.4
1	B	896	ASP	11.4
1	B	2218	GLY	11.4
1	B	2126	ILE	11.3
1	A	1167	ARG	11.3
1	A	864	LEU	11.3
1	B	948	GLU	11.3
1	A	1290	VAL	11.2

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Mol	Chain	Res	Type	RSRZ
1	B	1257	VAL	11.2
1	B	878	GLN	11.2
1	B	791	VAL	11.2
1	A	1103	GLU	11.1
1	B	1254	VAL	11.1
1	A	847	ALA	11.1
1	A	1170	SER	11.0
1	B	792	VAL	11.0
1	B	882	VAL	11.0
1	B	1684	PHE	10.9
1	B	1191	ILE	10.9
1	B	892	PRO	10.9
1	A	1701	LEU	10.9
1	A	2123	LEU	10.9
1	A	2119	ARG	10.9
1	A	1691	PRO	10.9
1	B	1730	ILE	10.9
1	A	930	LEU	10.8
1	B	968	THR	10.8
1	B	860	LEU	10.7
1	B	1255	VAL	10.7
1	A	1004	ARG	10.6
1	A	1007	LEU	10.6
1	B	904	LEU	10.6
1	A	1254	VAL	10.5
1	B	1192	VAL	10.5
1	A	1695	GLU	10.5
1	A	1101	ALA	10.4
1	A	2001	GLN	10.3
1	A	1700	TYR	10.3
1	B	2220	PRO	10.3
1	B	2129	GLN	10.3
1	B	2228	GLU	10.3
1	B	793	GLY	10.3
1	B	1253	ALA	10.3
1	A	1698	PHE	10.2
1	B	2089	ASP	10.2
1	B	844	GLN	10.2
1	B	848	LEU	10.2
1	B	918	GLN	10.2
1	A	1256	ASN	10.2
1	A	860	LEU	10.2

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Mol	Chain	Res	Type	RSRZ
1	B	846	SER	10.2
1	A	989	TYR	10.1
1	A	1692	ALA	10.1
1	B	1102	LEU	10.0
1	B	2219	ILE	10.0
1	A	2092	TYR	10.0
1	A	839	SER	10.0
1	A	840	GLU	10.0
1	B	790	VAL	10.0
1	A	1008	ARG	10.0
1	A	861	THR	9.9
1	B	1155	SER	9.9
1	B	1189	GLY	9.9
1	B	837	PRO	9.9
1	A	2098	GLU	9.9
1	B	840	GLU	9.9
1	A	834	PRO	9.8
1	A	2127	TYR	9.7
1	A	1704	SER	9.7
1	A	999	VAL	9.7
1	A	927	ALA	9.7
1	B	949	GLU	9.7
1	B	2133	GLN	9.7
1	A	1005	PRO	9.7
1	A	790	VAL	9.6
1	B	845	PHE	9.6
1	B	907	LEU	9.6
1	A	1683	HIS	9.5
1	B	1188	LYS	9.5
1	A	857	ASP	9.5
1	A	1730	ILE	9.5
1	A	1029	LEU	9.5
1	A	1292	ARG	9.5
1	A	824	LEU	9.4
1	B	936	VAL	9.4
1	A	1723	ASP	9.4
1	B	2132	VAL	9.3
1	A	986	LEU	9.3
1	B	2122	LEU	9.3
1	A	1306	SER	9.3
1	B	1676	LEU	9.2
1	B	884	ASN	9.2

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Mol	Chain	Res	Type	RSRZ
1	B	872	ALA	9.2
1	B	955	ARG	9.2
1	A	947	ASP	9.1
1	B	1475	LEU	9.1
1	A	789	PRO	9.1
1	A	992	ASN	9.1
1	A	1161	VAL	9.1
1	A	948	GLU	9.0
1	B	873	GLU	9.0
1	A	833	ASP	9.0
1	B	2134	PHE	9.0
1	B	937	GLU	8.9
1	A	929	LEU	8.9
1	B	851	ARG	8.9
1	A	1190	VAL	8.9
1	A	873	GLU	8.9
1	A	1305	PRO	8.8
1	B	972	HIS	8.8
1	A	1707	ALA	8.8
1	B	863	VAL	8.8
1	B	2119	ARG	8.8
1	A	982	VAL	8.8
1	A	1291	ARG	8.8
1	B	1494	GLU	8.7
1	B	2173	GLU	8.7
1	A	1177	LEU	8.7
1	A	875	PRO	8.7
1	A	1006	VAL	8.7
1	A	1191	ILE	8.7
1	A	925	LEU	8.7
1	B	2196	ASN	8.7
1	A	988	GLU	8.6
1	A	2090	PRO	8.6
1	B	2087	ARG	8.6
1	B	2169	ARG	8.6
1	B	834	PRO	8.6
1	A	2130	ILE	8.6
1	A	2187	ALA	8.6
1	B	2197	THR	8.6
1	B	2085	MET	8.6
1	B	876	ALA	8.6
1	B	2249	LYS	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	1255	VAL	8.6
1	A	1102	LEU	8.6
1	A	2084	THR	8.5
1	B	877	ARG	8.5
1	B	856	LEU	8.5
1	A	858	ALA	8.5
1	A	1000	GLY	8.5
1	B	2226	ASP	8.5
1	A	1296	ILE	8.5
1	A	2134	PHE	8.5
1	A	2259	LEU	8.4
1	A	1675	GLY	8.4
1	B	1683	HIS	8.4
1	A	1929	PRO	8.4
1	A	836	LEU	8.4
1	B	1677	ALA	8.3
1	A	2116	MET	8.3
1	A	879	LEU	8.3
1	B	1702	TYR	8.3
1	B	1129	ILE	8.3
1	B	1211	LEU	8.3
1	B	939	GLN	8.3
1	A	827	PHE	8.3
1	A	938	CYS	8.2
1	B	2243	LYS	8.2
1	A	940	PHE	8.2
1	B	1680	LEU	8.2
1	A	1183	ASP	8.2
1	B	843	ALA	8.2
1	B	2221	GLY	8.2
1	A	2091	VAL	8.2
1	B	1164	ASP	8.2
1	A	1722	GLU	8.2
1	A	1999	GLY	8.1
1	A	945	LEU	8.1
1	A	2131	CYS	8.1
1	B	1258	ALA	8.0
1	A	968	THR	8.0
1	B	847	ALA	8.0
1	A	835	LYS	8.0
1	B	1460	ASN	8.0
1	B	1203	ALA	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	949	GLU	8.0
1	A	848	LEU	8.0
1	B	952	LEU	8.0
1	A	1676	LEU	7.9
1	A	884	ASN	7.9
1	A	1016	ARG	7.9
1	A	1297	CYS	7.9
1	B	1293	LEU	7.9
1	B	2135	ALA	7.9
1	A	1178	ALA	7.9
1	A	828	ILE	7.9
1	B	1169	HIS	7.9
1	A	850	ALA	7.9
1	A	893	ASN	7.8
1	A	843	ALA	7.8
1	A	2099	MET	7.8
1	A	844	GLN	7.8
1	B	1290	VAL	7.8
1	A	1619	PRO	7.8
1	B	1715	VAL	7.8
1	A	2095	LEU	7.8
1	A	907	LEU	7.8
1	B	2166	ARG	7.7
1	B	864	LEU	7.7
1	A	937	GLU	7.7
1	B	1131	TRP	7.7
1	B	2222	PHE	7.7
1	A	1015	SER	7.7
1	A	856	LEU	7.6
1	B	914	TYR	7.6
1	A	2203	PRO	7.6
1	A	1690	ASP	7.6
1	A	1304	TYR	7.6
1	A	2164	TYR	7.6
1	B	2213	LEU	7.6
1	A	1164	ASP	7.5
1	A	854	HIS	7.5
1	B	2124	LEU	7.5
1	A	1693	LYS	7.5
1	B	1675	GLY	7.5
1	B	965	VAL	7.5
1	A	2122	LEU	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	793	GLY	7.5
1	A	888	ASP	7.5
1	B	883	PHE	7.5
1	A	1187	ARG	7.5
1	B	1106	VAL	7.5
1	B	961	ASN	7.5
1	B	2128	HIS	7.5
1	A	1689	ASN	7.4
1	B	1187	ARG	7.4
1	B	933	TYR	7.4
1	A	1100	ALA	7.4
1	A	1028	VAL	7.4
1	A	1001	LYS	7.4
1	A	1105	TYR	7.4
1	A	1257	VAL	7.4
1	B	1284	ASP	7.4
1	B	940	PHE	7.4
1	A	2112	ILE	7.4
1	A	816	ASN	7.3
1	B	1703	LEU	7.3
1	B	1130	ASP	7.3
1	A	951	ILE	7.3
1	B	833	ASP	7.3
1	A	944	ARG	7.3
1	B	1732	THR	7.3
1	A	855	LYS	7.3
1	A	2102	GLU	7.2
1	A	1703	LEU	7.2
1	B	2125	PRO	7.2
1	B	2232	TRP	7.2
1	B	838	TYR	7.2
1	A	2138	HIS	7.2
1	A	1002	HIS	7.2
1	A	1058	GLY	7.2
1	B	794	SER	7.2
1	A	2133	GLN	7.2
1	B	1476	ARG	7.2
1	A	2103	GLY	7.1
1	B	881	LYS	7.1
1	B	1619	PRO	7.1
1	B	921	ARG	7.1
1	A	872	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	2224	THR	7.1
1	A	1009	ARG	7.1
1	A	984	ALA	7.1
1	B	1205	SER	7.1
1	A	1086	LEU	7.1
1	A	2064	GLY	7.1
1	A	2017	ASP	7.1
1	A	1576	PRO	7.0
1	A	1104	VAL	7.0
1	A	941	SER	7.0
1	B	831	LEU	7.0
1	B	1687	ALA	7.0
1	A	1351	ASN	7.0
1	B	2253	ALA	6.9
1	A	924	ASN	6.9
1	B	2227	ARG	6.9
1	B	1201	GLU	6.9
1	B	1154	PRO	6.9
1	B	1700	TYR	6.9
1	A	807	MET	6.9
1	B	1202	GLU	6.9
1	B	2223	LYS	6.9
1	A	1156	SER	6.8
1	A	2086	ALA	6.8
1	B	1153	VAL	6.8
1	A	1017	GLN	6.8
1	B	1704	SER	6.8
1	B	2259	LEU	6.8
1	A	933	TYR	6.8
1	A	1928	ILE	6.8
1	B	900	LEU	6.8
1	A	882	VAL	6.8
1	B	1473	MET	6.8
1	A	981	LEU	6.7
1	A	2087	ARG	6.7
1	B	1733	ILE	6.7
1	A	876	ALA	6.7
1	B	2233	TYR	6.7
1	A	995	ASN	6.7
1	A	1176	TYR	6.7
1	A	2104	LEU	6.7
1	B	2017	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	1010	LEU	6.7
1	A	2173	GLU	6.7
1	A	1153	VAL	6.6
1	A	934	ALA	6.6
1	A	1160	PRO	6.6
1	A	1162	GLU	6.6
1	A	883	PHE	6.6
1	B	2230	VAL	6.5
1	A	979	ASN	6.5
1	A	2054	GLU	6.5
1	B	2084	THR	6.5
1	A	1927	GLY	6.5
1	B	1681	MET	6.5
1	A	1680	LEU	6.5
1	A	1699	LYS	6.5
1	B	1948	PRO	6.5
1	B	888	ASP	6.5
1	A	1727	ARG	6.5
1	B	1200	ALA	6.5
1	B	1695	GLU	6.5
1	A	2111	ASN	6.5
1	A	1180	ARG	6.5
1	A	859	GLN	6.4
1	A	2063	GLY	6.4
1	A	889	ASP	6.4
1	A	868	GLN	6.4
1	B	2214	GLU	6.4
1	A	1295	PHE	6.4
1	B	839	SER	6.4
1	A	942	GLY	6.4
1	A	980	SER	6.4
1	B	2245	GLU	6.4
1	A	1158	ALA	6.3
1	A	936	VAL	6.3
1	B	800	PHE	6.3
1	B	836	LEU	6.3
1	A	1705	ASP	6.3
1	B	1723	ASP	6.3
1	B	1288	ARG	6.3
1	A	1474	PRO	6.3
1	B	886	PHE	6.3
1	B	1285	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	1293	LEU	6.3
1	A	1494	GLU	6.3
1	B	2225	ASN	6.2
1	B	796	PRO	6.2
1	A	885	LYS	6.2
1	B	1204	LEU	6.2
1	A	2217	VAL	6.2
1	A	1724	GLY	6.2
1	A	1372	ALA	6.2
1	B	969	VAL	6.2
1	A	1850	ILE	6.2
1	B	1163	ASN	6.2
1	B	951	ILE	6.2
1	B	2165	TRP	6.2
1	A	1025	ALA	6.2
1	A	1173	ASP	6.2
1	A	1697	GLY	6.2
1	A	1087	THR	6.2
1	B	1301	ASP	6.2
1	B	849	HIS	6.1
1	A	1925	LEU	6.1
1	B	1127	TYR	6.1
1	A	2176	ILE	6.1
1	B	2246	LYS	6.1
1	A	2121	GLU	6.1
1	A	2206	ARG	6.1
1	A	1106	VAL	6.1
1	A	829	GLU	6.1
1	B	895	THR	6.1
1	A	921	ARG	6.1
1	B	799	ARG	6.1
1	A	2167	VAL	6.1
1	A	1193	PRO	6.1
1	A	1018	SER	6.1
1	B	2204	GLU	6.1
1	A	2105	SER	6.1
1	A	2096	LYS	6.1
1	A	2163	PHE	6.0
1	A	1574	LYS	6.0
1	B	2020	THR	6.0
1	A	865	GLU	6.0
1	B	1424	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	923	LEU	6.0
1	A	1677	ALA	6.0
1	A	911	LEU	6.0
1	B	789	PRO	6.0
1	A	890	ASN	6.0
1	B	1688	TRP	6.0
1	A	1323	HIS	6.0
1	A	2166	ARG	6.0
1	A	2109	SER	6.0
1	A	1307	TYR	6.0
1	A	912	ASN	6.0
1	A	952	LEU	6.0
1	B	2120	GLU	6.0
1	A	1154	PRO	6.0
1	B	1310	PHE	5.9
1	B	1294	THR	5.9
1	A	1561	TRP	5.9
1	B	973	LYS	5.9
1	B	917	GLY	5.9
1	B	1678	GLU	5.9
1	A	969	VAL	5.9
1	A	1308	TYR	5.9
1	A	2115	LYS	5.9
1	A	796	PRO	5.9
1	B	1725	GLU	5.9
1	A	1725	GLU	5.9
1	B	2159	SER	5.9
1	B	1099	LEU	5.9
1	B	1717	THR	5.9
1	A	914	TYR	5.9
1	A	2082	LEU	5.8
1	A	794	SER	5.8
1	A	1572	ALA	5.8
1	A	853	PRO	5.8
1	B	1694	PRO	5.8
1	A	1717	THR	5.8
1	A	955	ARG	5.8
1	A	950	ALA	5.8
1	A	1185	PRO	5.8
1	B	2239	ARG	5.8
1	A	2093	ARG	5.8
1	A	987	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	1110	TYR	5.8
1	A	997	GLY	5.8
1	A	2000	GLY	5.8
1	B	1728	HIS	5.8
1	A	1011	THR	5.8
1	A	953	LYS	5.8
1	A	1090	PHE	5.8
1	A	2117	GLN	5.7
1	A	983	LEU	5.7
1	A	2108	GLU	5.7
1	B	832	ARG	5.7
1	B	974	ASN	5.7
1	B	1726	LYS	5.7
1	B	1876	PRO	5.7
1	B	889	ASP	5.7
1	B	967	ASN	5.7
1	A	1930	MET	5.7
1	A	886	PHE	5.7
1	B	985	LEU	5.7
1	B	2256	MET	5.7
1	A	878	GLN	5.7
1	B	835	LYS	5.7
1	B	2215	SER	5.7
1	B	2172	ILE	5.7
1	A	2233	TYR	5.7
1	A	972	HIS	5.6
1	B	2250	GLU	5.6
1	A	792	VAL	5.6
1	A	2168	ARG	5.6
1	B	807	MET	5.6
1	A	2256	MET	5.6
1	B	1186	ILE	5.6
1	A	851	ARG	5.6
1	A	2204	GLU	5.6
1	A	1715	VAL	5.6
1	B	1618	THR	5.6
1	B	2081	GLN	5.6
1	A	967	ASN	5.6
1	A	1312	GLY	5.6
1	B	2210	LEU	5.6
1	A	831	LEU	5.6
1	B	2176	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	1618	THR	5.6
1	A	862	GLN	5.6
1	B	2164	TYR	5.6
1	B	1193	PRO	5.5
1	A	2118	GLN	5.5
1	A	1861	LEU	5.5
1	A	1159	THR	5.5
1	A	1325	GLU	5.5
1	B	957	GLN	5.5
1	B	2261	ARG	5.5
1	A	2165	TRP	5.5
1	B	818	VAL	5.5
1	B	2247	LEU	5.5
1	B	1160	PRO	5.5
1	B	2155	GLN	5.5
1	B	1179	ARG	5.5
1	A	1020	LYS	5.5
1	B	1459	ILE	5.5
1	A	1012	GLU	5.5
1	B	1291	ARG	5.5
1	A	2170	ARG	5.4
1	A	1706	GLU	5.4
1	A	1044	MET	5.4
1	A	2216	TRP	5.4
1	B	1104	VAL	5.4
1	B	2157	ARG	5.4
1	B	1729	LYS	5.4
1	A	2159	SER	5.4
1	A	910	VAL	5.4
1	B	1208	LEU	5.4
1	B	867	ALA	5.4
1	A	998	ASN	5.4
1	A	2094	SER	5.4
1	B	1105	TYR	5.4
1	B	1974	ALA	5.4
1	A	1860	ILE	5.4
1	B	922	GLU	5.4
1	A	2232	TRP	5.4
1	A	1476	ARG	5.4
1	B	2244	LEU	5.4
1	A	1658	LYS	5.4
1	A	881	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	795	LYS	5.3
1	B	2168	ARG	5.3
1	A	1179	ARG	5.3
1	B	1296	ILE	5.3
1	A	1879	LYS	5.3
1	B	817	GLN	5.3
1	B	1295	PHE	5.3
1	A	1289	ARG	5.3
1	A	1021	VAL	5.3
1	B	1167	ARG	5.3
1	A	1285	LEU	5.3
1	A	1864	SER	5.3
1	A	863	VAL	5.3
1	A	2135	ALA	5.3
1	A	825	LYS	5.3
1	A	830	VAL	5.3
1	A	1363	GLU	5.3
1	B	971	SER	5.3
1	B	982	VAL	5.3
1	B	1133	PHE	5.3
1	A	931	SER	5.3
1	A	817	GLN	5.3
1	A	1573	ALA	5.2
1	B	1101	ALA	5.2
1	A	1026	ARG	5.2
1	A	2013	SER	5.2
1	A	2124	LEU	5.2
1	A	1294	THR	5.2
1	B	859	GLN	5.2
1	B	1760	ASN	5.2
1	A	800	PHE	5.2
1	B	1119	ARG	5.2
1	A	2018	ALA	5.2
1	A	928	ASP	5.2
1	A	1354	VAL	5.2
1	A	2162	PHE	5.2
1	B	2252	ILE	5.2
1	B	1461	CYS	5.2
1	A	1931	GLY	5.2
1	B	2018	ALA	5.2
1	A	978	LYS	5.1
1	B	1113	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	906	PRO	5.1
1	A	2113	LYS	5.1
1	A	1353	HIS	5.1
1	B	1865	PRO	5.1
1	A	1756	SER	5.1
1	A	1734	VAL	5.1
1	B	935	ASP	5.1
1	B	1170	SER	5.1
1	B	930	LEU	5.1
1	A	1014	GLU	5.1
1	B	1370	THR	5.1
1	B	2138	HIS	5.1
1	B	899	LEU	5.1
1	B	855	LYS	5.0
1	B	1864	SER	5.0
1	B	830	VAL	5.0
1	A	1085	VAL	5.0
1	B	2156	TRP	5.0
1	B	2021	ARG	5.0
1	A	1057	TYR	5.0
1	A	1620	GLU	5.0
1	B	1795	ILE	5.0
1	B	2231	GLU	5.0
1	B	890	ASN	5.0
1	B	891	VAL	5.0
1	B	1207	ALA	5.0
1	B	1018	SER	5.0
1	A	1729	LYS	5.0
1	A	1258	ALA	5.0
1	B	910	VAL	4.9
1	B	1118	VAL	4.9
1	B	964	LYS	4.9
1	B	2260	LEU	4.9
1	B	926	ILE	4.9
1	A	1987	PRO	4.9
1	B	2174	ASP	4.9
1	A	1728	HIS	4.9
1	A	1423	HIS	4.9
1	B	2248	LYS	4.9
1	B	1817	LEU	4.9
1	A	1303	SER	4.9
1	B	1292	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1726	LYS	4.8
1	A	1475	LEU	4.8
1	B	2170	ARG	4.8
1	A	1732	THR	4.8
1	A	1859	PRO	4.8
1	B	1100	ALA	4.8
1	B	1818	GLY	4.8
1	A	1192	VAL	4.8
1	B	827	PHE	4.8
1	A	2056	TYR	4.8
1	B	911	LEU	4.8
1	B	2240	ILE	4.8
1	B	2187	ALA	4.8
1	B	1493	GLU	4.8
1	A	1681	MET	4.8
1	A	1863	PRO	4.8
1	B	1714	GLU	4.8
1	A	803	LEU	4.8
1	A	2081	GLN	4.8
1	A	2107	GLU	4.8
1	B	2013	SER	4.8
1	B	978	LYS	4.8
1	A	1109	ALA	4.8
1	B	966	VAL	4.8
1	A	1733	ILE	4.8
1	B	988	GLU	4.7
1	A	954	LEU	4.7
1	B	938	CYS	4.7
1	A	1182	ARG	4.7
1	A	1924	ARG	4.7
1	B	1458	ARG	4.7
1	B	1727	ARG	4.7
1	A	1350	LYS	4.7
1	B	803	LEU	4.7
1	A	806	THR	4.7
1	B	1698	PHE	4.7
1	B	2068	PRO	4.7
1	B	880	LEU	4.7
1	B	1199	ASP	4.7
1	B	1734	VAL	4.7
1	A	1696	ALA	4.7
1	B	897	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1115	LEU	4.7
1	A	823	LYS	4.7
1	A	1577	ALA	4.7
1	B	1875	THR	4.7
1	B	2163	PHE	4.7
1	A	815	ASP	4.7
1	B	1183	ASP	4.7
1	A	1019	ALA	4.7
1	A	2126	ILE	4.7
1	B	989	TYR	4.7
1	A	2075	LYS	4.7
1	A	2125	PRO	4.7
1	A	1175	THR	4.6
1	A	990	ARG	4.6
1	B	1194	CYS	4.6
1	B	1679	GLU	4.6
1	A	821	GLN	4.6
1	A	1084	ASP	4.6
1	B	1472	THR	4.6
1	B	2086	ALA	4.6
1	B	850	ALA	4.6
1	B	887	LEU	4.6
1	B	1872	VAL	4.6
1	B	2167	VAL	4.6
1	A	2169	ARG	4.6
1	A	894	LYS	4.6
1	A	1521	VAL	4.6
1	B	1423	HIS	4.6
1	B	1692	ALA	4.6
1	A	1711	PHE	4.6
1	A	916	ASP	4.6
1	A	2020	THR	4.6
1	A	965	VAL	4.6
1	A	2255	GLN	4.6
1	B	1947	ASP	4.6
1	A	943	ARG	4.6
1	B	1731	ILE	4.6
1	B	1742	VAL	4.6
1	A	1024	LYS	4.6
1	A	922	GLU	4.6
1	A	877	ARG	4.5
1	B	2090	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	1620	GLU	4.5
1	A	869	ASN	4.5
1	A	1742	VAL	4.5
1	B	868	GLN	4.5
1	B	2016	VAL	4.5
1	A	1984	GLU	4.5
1	B	1165	PHE	4.5
1	A	935	ASP	4.5
1	B	1978	ASN	4.5
1	B	956	ASP	4.5
1	A	1027	GLU	4.5
1	B	2162	PHE	4.5
1	B	1426	GLN	4.5
1	B	2255	GLN	4.5
1	A	2100	ALA	4.5
1	B	1981	ASN	4.4
1	B	1863	PRO	4.4
1	B	1477	VAL	4.4
1	A	1083	PHE	4.4
1	A	1862	SER	4.4
1	A	918	GLN	4.4
1	A	908	THR	4.4
1	A	804	TYR	4.4
1	A	996	VAL	4.4
1	B	2212	GLN	4.4
1	B	1371	ARG	4.4
1	A	1362	VAL	4.4
1	B	2092	TYR	4.4
1	B	2258	GLU	4.4
1	A	1483	SER	4.4
1	B	2012	GLY	4.4
1	B	970	LEU	4.4
1	A	2207	SER	4.4
1	A	887	LEU	4.4
1	B	1416	HIS	4.4
1	B	1212	PRO	4.3
1	A	2106	LYS	4.3
1	B	1705	ASP	4.3
1	A	2076	TYR	4.3
1	A	1310	PHE	4.3
1	B	2076	TYR	4.3
1	A	1493	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1902	PHE	4.3
1	B	1861	LEU	4.3
1	A	1760	ASN	4.3
1	A	1903	ASP	4.3
1	A	917	GLY	4.3
1	A	1682	PRO	4.3
1	A	1030	ILE	4.3
1	A	1299	ARG	4.3
1	A	1741	GLY	4.3
1	B	944	ARG	4.3
1	B	2049	ASN	4.3
1	A	1926	GLY	4.3
1	B	2158	GLN	4.3
1	A	904	LEU	4.3
1	A	1848	SER	4.3
1	B	1575	GLN	4.3
1	A	826	GLU	4.3
1	A	1373	VAL	4.3
1	B	1464	SER	4.3
1	B	1168	ILE	4.2
1	A	2229	VAL	4.2
1	B	1722	GLU	4.2
1	B	1126	PRO	4.2
1	B	1691	PRO	4.2
1	B	1124	GLU	4.2
1	A	2257	ARG	4.2
1	A	1288	ARG	4.2
1	B	1289	ARG	4.2
1	B	2082	LEU	4.2
1	A	1714	GLU	4.2
1	A	880	LEU	4.2
1	A	1110	TYR	4.2
1	A	971	SER	4.2
1	A	2197	THR	4.2
1	B	1206	ARG	4.2
1	B	1603	GLY	4.2
1	B	929	LEU	4.1
1	B	1719	GLU	4.1
1	A	832	ARG	4.1
1	B	1596	ALA	4.1
1	A	1735	GLY	4.1
1	A	2114	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1286	LEU	4.1
1	A	892	PRO	4.1
1	A	960	ASP	4.1
1	A	1719	GLU	4.1
1	A	977	SER	4.1
1	A	1031	LEU	4.1
1	B	1693	LYS	4.1
1	B	1429	ALA	4.1
1	B	1756	SER	4.1
1	B	1197	LEU	4.1
1	A	1901	LEU	4.1
1	B	1741	GLY	4.1
1	A	2097	LYS	4.1
1	A	795	LYS	4.1
1	A	913	LEU	4.1
1	A	2198	SER	4.1
1	A	2210	LEU	4.0
1	B	2254	ASP	4.1
1	A	1324	ILE	4.0
1	A	1865	PRO	4.0
1	B	1210	VAL	4.0
1	B	981	LEU	4.0
1	A	1522	SER	4.0
1	A	1708	LYS	4.0
1	A	1311	ARG	4.0
1	B	1297	CYS	4.0
1	A	1880	GLN	4.0
1	B	1161	VAL	4.0
1	B	813	GLY	4.0
1	A	973	LYS	4.0
1	B	925	LEU	4.0
1	B	995	ASN	4.0
1	B	1899	PRO	4.0
1	B	2257	ARG	4.0
1	B	2023	GLU	4.0
1	B	1158	ALA	4.0
1	B	902	SER	4.0
1	B	2143	ARG	4.0
1	A	1165	PHE	4.0
1	B	1369	PHE	4.0
1	A	2027	PHE	4.0
1	B	2203	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1757	ARG	4.0
1	B	979	ASN	4.0
1	B	885	LYS	4.0
1	A	1298	GLY	3.9
1	B	828	ILE	3.9
1	A	909	SER	3.9
1	A	1211	LEU	3.9
1	A	1622	PRO	3.9
1	B	975	VAL	3.9
1	B	953	LYS	3.9
1	A	2137	LEU	3.9
1	B	1120	TYR	3.9
1	B	1735	GLY	3.9
1	A	1069	ARG	3.9
1	A	1259	VAL	3.9
1	B	1546	VAL	3.9
1	A	1459	ILE	3.9
1	A	905	GLU	3.9
1	A	1040	ARG	3.9
1	B	1716	ILE	3.9
1	A	2110	ASP	3.9
1	A	932	MET	3.9
1	A	2222	PHE	3.9
1	A	2140	ARG	3.9
1	B	1816	GLN	3.9
1	A	1022	SER	3.9
1	B	1178	ALA	3.9
1	B	1125	ARG	3.9
1	B	1463	ARG	3.9
1	A	1376	PRO	3.8
1	B	960	ASP	3.8
1	A	2177	LEU	3.8
1	A	2180	ILE	3.8
1	A	797	ALA	3.8
1	A	867	ALA	3.8
1	B	1949	ALA	3.8
1	A	2160	ARG	3.8
1	B	905	GLU	3.8
1	B	1122	ASP	3.8
1	A	1099	LEU	3.8
1	B	1887	MET	3.8
1	B	797	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	2025	PRO	3.8
1	A	2258	GLU	3.8
1	A	1013	LEU	3.8
1	B	1092	HIS	3.8
1	B	1979	ASP	3.8
1	B	2091	VAL	3.8
1	A	1287	ALA	3.8
1	B	857	ASP	3.8
1	B	986	LEU	3.8
1	B	916	ASP	3.8
1	B	1308	TYR	3.8
1	A	1502	TRP	3.8
1	A	1174	MET	3.8
1	A	1905	ASP	3.8
1	A	1464	SER	3.8
1	B	824	LEU	3.8
1	A	852	MET	3.8
1	A	1429	ALA	3.8
1	A	1868	TRP	3.8
1	A	1934	ALA	3.8
1	B	1176	TYR	3.8
1	A	2083	GLU	3.8
1	B	1017	GLN	3.7
1	A	2141	ALA	3.7
1	B	1873	VAL	3.7
1	B	1456	GLU	3.7
1	A	963	GLN	3.7
1	A	1560	SER	3.7
1	B	1868	TRP	3.7
1	B	2118	GLN	3.7
1	A	2236	ASN	3.7
1	A	1858	LEU	3.7
1	B	811	LEU	3.7
1	A	966	VAL	3.7
1	A	788	SER	3.7
1	A	811	LEU	3.7
1	B	861	THR	3.7
1	B	1761	ASP	3.7
1	B	1945	PRO	3.7
1	A	1529	ASN	3.7
1	B	2015	ILE	3.7
1	B	1707	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	799	ARG	3.6
1	A	964	LYS	3.6
1	B	1597	GLU	3.6
1	A	818	VAL	3.6
1	B	954	LEU	3.6
1	A	1364	THR	3.6
1	A	2213	LEU	3.6
1	B	1855	ASN	3.6
1	A	2143	ARG	3.6
1	A	1212	PRO	3.6
1	B	1021	VAL	3.6
1	A	1721	VAL	3.6
1	B	2251	SER	3.6
1	B	1862	SER	3.6
1	B	1724	GLY	3.6
1	A	1048	LEU	3.6
1	B	1720	ILE	3.6
1	B	1874	TYR	3.6
1	A	1847	LEU	3.6
1	A	1469	GLU	3.6
1	B	2209	HIS	3.6
1	B	2198	SER	3.6
1	B	2121	GLU	3.6
1	A	2041	TRP	3.6
1	A	1923	ALA	3.6
1	B	1612	TRP	3.6
1	A	820	MET	3.5
1	B	977	SER	3.6
1	B	2206	ARG	3.5
1	B	1198	LEU	3.5
1	B	1560	SER	3.5
1	A	1989	MET	3.5
1	B	2025	PRO	3.5
1	A	1347	THR	3.5
1	B	1588	VAL	3.5
1	B	1121	HIS	3.5
1	A	1849	PHE	3.5
1	A	1906	SER	3.5
1	A	805	GLY	3.5
1	B	950	ALA	3.5
1	B	1372	ALA	3.5
1	B	823	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	919	LYS	3.5
1	B	963	GLN	3.5
1	B	991	PRO	3.5
1	B	1184	GLU	3.4
1	A	2021	ARG	3.4
1	B	1900	GLY	3.4
1	B	1635	THR	3.4
1	A	1564	ALA	3.4
1	A	1309	THR	3.4
1	B	898	ASP	3.4
1	B	1811	TYR	3.4
1	A	1720	ILE	3.4
1	B	801	ALA	3.4
1	B	1492	TYR	3.4
1	A	2171	LEU	3.4
1	B	1417	MET	3.4
1	B	1784	GLN	3.4
1	B	1708	LYS	3.4
1	A	2139	ASP	3.4
1	A	991	PRO	3.4
1	A	2228	GLU	3.4
1	A	2062	ARG	3.3
1	A	2172	ILE	3.3
1	B	854	HIS	3.3
1	A	898	ASP	3.3
1	B	1718	GLU	3.3
1	B	1866	ASP	3.3
1	B	1975	GLN	3.3
1	B	901	LYS	3.3
1	A	801	ALA	3.3
1	A	2004	MET	3.3
1	B	2137	LEU	3.3
1	A	1355	TYR	3.3
1	B	908	THR	3.3
1	B	1793	PRO	3.3
1	A	1113	TYR	3.3
1	A	822	GLN	3.3
1	A	2132	VAL	3.3
1	B	1517	HIS	3.3
1	B	1016	ARG	3.3
1	A	956	ASP	3.3
1	A	1557	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2003	ASP	3.3
1	B	2054	GLU	3.3
1	B	1627	PHE	3.3
1	A	2128	HIS	3.3
1	A	1322	ARG	3.3
1	A	2239	ARG	3.3
1	A	798	GLN	3.3
1	B	2146	ALA	3.3
1	B	2069	GLU	3.3
1	A	1410	ASN	3.3
1	B	1931	GLY	3.3
1	B	1114	ASN	3.3
1	A	1172	SER	3.3
1	A	1991	LEU	3.3
1	B	2177	LEU	3.3
1	A	1482	THR	3.2
1	B	2142	GLY	3.2
1	B	2022	PHE	3.2
1	B	1598	VAL	3.2
1	A	1274	ILE	3.2
1	B	947	ASP	3.2
1	B	1576	PRO	3.2
1	B	1010	LEU	3.2
1	A	1375	ARG	3.2
1	A	1345	VAL	3.2
1	B	1159	THR	3.2
1	A	2209	HIS	3.2
1	B	1721	VAL	3.2
1	A	1495	LYS	3.2
1	B	2065	VAL	3.2
1	A	961	ASN	3.2
1	A	1678	GLU	3.2
1	B	1696	ALA	3.2
1	A	1313	PRO	3.2
1	B	1699	LYS	3.2
1	A	1679	GLU	3.2
1	A	2002	ARG	3.2
1	B	1483	SER	3.2
1	B	946	GLN	3.2
1	A	1543	THR	3.2
1	B	870	ARG	3.2
1	B	2186	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2244	LEU	3.2
1	B	1491	LEU	3.2
1	A	802	VAL	3.2
1	A	1082	VAL	3.2
1	A	2230	VAL	3.2
1	B	2116	MET	3.2
1	B	2144	MET	3.2
1	A	1836	ASP	3.2
1	B	1196	ASP	3.2
1	A	970	LEU	3.1
1	A	1264	GLY	3.1
1	B	1259	VAL	3.1
1	A	2174	ASP	3.1
1	B	1306	SER	3.1
1	B	1543	THR	3.1
1	A	1932	VAL	3.1
1	A	915	LEU	3.1
1	B	1587	LEU	3.1
1	B	1123	GLU	3.1
1	B	1495	LYS	3.1
1	B	1794	ILE	3.1
1	A	1315	TYR	3.1
1	A	1986	LEU	3.1
1	A	2179	ARG	3.1
1	B	2160	ARG	3.1
1	B	2207	SER	3.1
1	A	2240	ILE	3.1
1	B	1682	PRO	3.1
1	A	1637	LYS	3.1
1	B	1427	VAL	3.1
1	B	1544	GLN	3.1
1	B	1286	LEU	3.1
1	B	862	GLN	3.1
1	B	804	TYR	3.1
1	B	871	GLY	3.1
1	A	975	VAL	3.1
1	A	1518	LEU	3.1
1	B	1711	PHE	3.1
1	A	808	CYS	3.1
1	A	1761	ASP	3.0
1	B	1132	ASP	3.0
1	A	2024	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1588	VAL	3.0
1	A	2101	LYS	3.0
1	B	959	LYS	3.0
1	A	2161	ARG	3.0
1	A	1558	GLN	3.0
1	B	1901	LEU	3.0
1	B	1985	GLN	3.0
1	A	810	ILE	3.0
1	A	1374	VAL	3.0
1	A	974	ASN	3.0
1	A	2219	ILE	3.0
1	B	1354	VAL	3.0
1	B	1592	GLN	3.0
1	A	1433	ALA	3.0
1	A	1900	GLY	3.0
1	B	1263	GLU	3.0
1	B	1156	SER	3.0
1	B	1471	ASP	3.0
1	B	942	GLY	3.0
1	B	1363	GLU	3.0
1	A	1197	LEU	3.0
1	A	1428	THR	3.0
1	B	1107	ARG	3.0
1	A	1320	SER	3.0
1	B	912	ASN	3.0
1	A	1562	THR	3.0
1	B	866	ARG	3.0
1	B	1637	LYS	3.0
1	B	1710	ARG	3.0
1	B	2019	LEU	3.0
1	A	1370	THR	2.9
1	B	1987	PRO	2.9
1	A	2129	GLN	2.9
1	B	1982	TYR	2.9
1	B	958	TYR	2.9
1	A	1710	ARG	2.9
1	B	1326	PRO	2.9
1	A	1075	VAL	2.9
1	A	1204	LEU	2.9
1	A	1544	GLN	2.9
1	B	1706	GLU	2.9
1	A	2227	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1336	ARG	2.9
1	B	1300	ASN	2.9
1	B	2241	ASN	2.9
1	A	901	LYS	2.9
1	B	1869	ASP	2.9
1	B	1574	LYS	2.9
1	B	1175	THR	2.9
1	B	1425	PHE	2.9
1	A	2252	ILE	2.9
1	B	962	ILE	2.9
1	A	1985	GLN	2.9
1	B	1867	PRO	2.9
1	A	2005	TYR	2.9
1	B	1454	GLN	2.9
1	B	2071	ILE	2.9
1	A	2243	LYS	2.9
1	A	1327	SER	2.9
1	B	943	ARG	2.9
1	A	1081	THR	2.9
1	A	866	ARG	2.9
1	A	1786	ALA	2.8
1	B	1038	GLU	2.8
1	A	906	PRO	2.8
1	A	994	PRO	2.8
1	A	2144	MET	2.8
1	A	2205	THR	2.8
1	B	1274	ILE	2.8
1	A	1059	GLU	2.8
1	A	1662	PRO	2.8
1	B	1871	ASP	2.8
1	B	1970	ALA	2.8
1	A	1866	ASP	2.8
1	A	1473	MET	2.8
1	B	806	THR	2.8
1	B	1117	GLU	2.8
1	A	1284	ASP	2.8
1	A	2136	ASP	2.8
1	B	1421	PHE	2.8
1	B	2171	LEU	2.8
1	A	1425	PHE	2.8
1	A	1047	ILE	2.8
1	A	920	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1098	ALA	2.8
1	B	1410	ASN	2.8
1	A	1189	GLY	2.8
1	B	1287	ALA	2.8
1	B	2180	ILE	2.8
1	B	1547	TYR	2.8
1	B	1518	LEU	2.8
1	A	1117	GLU	2.8
1	B	1209	GLU	2.8
1	B	1338	SER	2.8
1	B	1181	THR	2.8
1	B	2032	PRO	2.8
1	A	2016	VAL	2.8
1	B	2179	ARG	2.8
1	B	1478	ILE	2.8
1	A	1846	TRP	2.7
1	B	1561	TRP	2.7
1	B	1356	GLU	2.7
1	B	1928	ILE	2.7
1	A	1542	GLY	2.7
1	B	1658	LYS	2.7
1	B	1581	CYS	2.7
1	A	812	ASN	2.7
1	B	2056	TYR	2.7
1	B	1586	GLU	2.7
1	A	1627	PHE	2.7
1	A	2049	ASN	2.7
1	A	1709	ARG	2.7
1	A	1887	MET	2.7
1	A	870	ARG	2.7
1	A	1617	ARG	2.7
1	A	1625	ARG	2.7
1	B	1128	PHE	2.7
1	A	1208	LEU	2.7
1	A	1079	LYS	2.7
1	B	1116	ARG	2.7
1	A	2078	LYS	2.7
1	A	2079	ASP	2.7
1	A	814	TYR	2.7
1	A	1546	VAL	2.7
1	B	1628	ILE	2.7
1	A	1133	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	919	LYS	2.7
1	A	1888	ILE	2.7
1	A	2153	SER	2.7
1	A	1430	ASP	2.7
1	B	2027	PHE	2.6
1	A	809	ASP	2.6
1	B	1422	SER	2.6
1	B	1505	TYR	2.6
1	A	1089	PHE	2.6
1	A	1361	GLY	2.6
1	B	865	GLU	2.6
1	B	1281	SER	2.6
1	B	1989	MET	2.6
1	B	1420	ASN	2.6
1	A	1088	LEU	2.6
1	A	1581	CYS	2.6
1	A	1763	PHE	2.6
1	A	1408	GLY	2.6
1	A	1753	GLY	2.6
1	B	1983	GLY	2.6
1	B	1622	PRO	2.6
1	A	1074	GLU	2.6
1	B	1515	SER	2.6
1	A	871	GLY	2.6
1	B	1600	ARG	2.6
1	B	1888	ILE	2.6
1	A	1571	LEU	2.6
1	A	1157	PRO	2.6
1	A	1344	PRO	2.6
1	A	1371	ARG	2.6
1	B	1044	MET	2.6
1	B	1759	TYR	2.6
1	A	2156	TRP	2.6
1	A	1107	ARG	2.5
1	A	1629	VAL	2.5
1	A	1188	LYS	2.5
1	B	1860	ILE	2.5
1	B	2072	ILE	2.5
1	B	1109	ALA	2.5
1	A	2036	LEU	2.5
1	A	1978	ASN	2.5
1	B	820	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1786	ALA	2.5
1	A	1379	LEU	2.5
1	B	1112	ALA	2.5
1	B	1736	ALA	2.5
1	A	2012	GLY	2.5
1	B	1697	GLY	2.5
1	B	1457	ILE	2.5
1	A	903	THR	2.5
1	A	1524	PRO	2.5
1	B	932	MET	2.5
1	B	1976	ALA	2.5
1	A	1904	LYS	2.5
1	B	812	ASN	2.5
1	B	1614	ILE	2.5
1	B	2115	LYS	2.5
1	A	813	GLY	2.5
1	B	1433	ALA	2.5
1	A	1369	PHE	2.5
1	B	1884	VAL	2.5
1	A	1851	PRO	2.5
1	A	891	VAL	2.5
1	B	2083	GLU	2.5
1	B	1926	GLY	2.5
1	B	1930	MET	2.5
1	A	1812	THR	2.5
1	A	1807	GLY	2.5
1	B	1025	ALA	2.5
1	B	1514	GLY	2.5
1	B	1870	ARG	2.5
1	B	1355	TYR	2.4
1	A	1321	ILE	2.4
1	B	2161	ARG	2.4
1	A	1166	LYS	2.4
1	A	1067	PRO	2.4
1	B	1616	ALA	2.4
1	A	1023	LEU	2.4
1	A	1933	ILE	2.4
1	A	2201	ALA	2.4
1	B	934	ALA	2.4
1	B	1378	ARG	2.4
1	A	1404	LEU	2.4
1	A	2055	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	798	GLN	2.4
1	B	915	LEU	2.4
1	B	1573	ALA	2.4
1	B	1934	ALA	2.4
1	A	1787	VAL	2.4
1	A	2231	GLU	2.4
1	B	819	VAL	2.4
1	B	826	GLU	2.4
1	B	1115	LEU	2.4
1	A	1055	SER	2.4
1	B	994	PRO	2.4
1	B	1545	TYR	2.4
1	A	2155	GLN	2.4
1	A	1080	TYR	2.4
1	A	2045	ASP	2.4
1	A	1716	ILE	2.4
1	B	1810	VAL	2.4
1	A	1041	THR	2.4
1	B	788	SER	2.4
1	B	2024	LYS	2.4
1	A	1628	ILE	2.4
1	B	2040	SER	2.4
1	B	2064	GLY	2.4
1	B	1462	MET	2.4
1	A	1326	PRO	2.4
1	A	1844	VAL	2.4
1	A	1592	GLN	2.4
1	A	819	VAL	2.4
1	A	2234	GLU	2.4
1	B	1373	VAL	2.4
1	B	1709	ARG	2.4
1	A	902	SER	2.4
1	A	1635	THR	2.4
1	B	1003	LEU	2.3
1	B	1315	TYR	2.3
1	B	1898	GLN	2.3
1	B	1737	GLU	2.3
1	B	2052	SER	2.3
1	B	1349	ASN	2.3
1	A	2253	ALA	2.3
1	A	2068	PRO	2.3
1	A	2057	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1525	TYR	2.3
1	A	1784	GLN	2.3
1	A	1876	PRO	2.3
1	B	1599	SER	2.3
1	A	1594	ASN	2.3
1	A	1993	ASN	2.3
1	A	2077	LYS	2.3
1	A	1078	SER	2.3
1	B	2014	PHE	2.3
1	A	1813	SER	2.3
1	A	2142	GLY	2.3
1	A	2202	SER	2.3
1	A	2226	ASP	2.3
1	B	1415	ASN	2.3
1	B	1611	GLY	2.3
1	B	810	ILE	2.3
1	B	1278	VAL	2.3
1	A	1319	ASP	2.3
1	A	1919	VAL	2.3
1	B	1844	VAL	2.3
1	A	1049	ARG	2.3
1	B	1013	LEU	2.3
1	A	1559	ASN	2.3
1	B	1582	ILE	2.3
1	B	1781	ARG	2.3
1	A	1596	ALA	2.3
1	A	2181	GLU	2.3
1	A	1368	TYR	2.3
1	A	2224	THR	2.3
1	B	1171	ILE	2.3
1	A	1664	ILE	2.3
1	B	2147	LYS	2.3
1	A	2235	GLN	2.2
1	A	1922	ARG	2.2
1	B	1521	VAL	2.2
1	B	1277	TRP	2.2
1	B	990	ARG	2.2
1	B	1006	VAL	2.2
1	B	1758	ALA	2.2
1	B	1098	ALA	2.2
1	B	1631	ALA	2.2
1	B	1904	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1755	THR	2.2
1	B	1399	ASP	2.2
1	A	1356	GLU	2.2
1	A	1491	LEU	2.2
1	B	1783	GLY	2.2
1	B	1594	ASN	2.2
1	A	1504	TYR	2.2
1	A	1755	THR	2.2
1	B	1364	THR	2.2
1	B	1629	VAL	2.2
1	B	1796	LEU	2.2
1	B	941	SER	2.2
1	B	1522	SER	2.2
1	A	1872	VAL	2.2
1	B	1996	GLY	2.2
1	B	1999	GLY	2.2
1	B	2051	ALA	2.2
1	B	2048	ILE	2.2
1	A	2225	ASN	2.2
1	A	1365	ASP	2.2
1	A	2200	ALA	2.2
1	B	1266	ASN	2.2
1	A	1461	CYS	2.2
1	A	2052	SER	2.2
1	B	2010	LYS	2.2
1	A	2186	PRO	2.2
1	B	1927	GLY	2.2
1	A	1956	GLN	2.2
1	B	1593	ASP	2.2
1	B	1753	GLY	2.2
1	A	1426	GLN	2.2
1	B	1764	THR	2.2
1	B	1746	ARG	2.2
1	B	987	ASP	2.2
1	A	959	LYS	2.2
1	A	1470	ASN	2.2
1	A	1974	ALA	2.2
1	B	2236	ASN	2.2
1	A	1409	THR	2.1
1	A	1377	GLY	2.1
1	B	1455	VAL	2.1
1	A	1736	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1477	VAL	2.1
1	A	1731	ILE	2.1
1	A	2028	ILE	2.1
1	A	1484	GLY	2.1
1	B	1950	ASN	2.1
1	A	895	THR	2.1
1	A	1330	PHE	2.1
1	A	1338	SER	2.1
1	B	1309	THR	2.1
1	A	1663	ARG	2.1
1	B	1946	ALA	2.1
1	A	1302	GLY	2.1
1	A	1545	TYR	2.1
1	A	1610	VAL	2.1
1	A	1568	ILE	2.1
1	A	1992	ALA	2.1
1	A	2157	ARG	2.1
1	B	1182	ARG	2.1
1	B	1082	VAL	2.1
1	B	1317	GLU	2.1
1	B	1157	PRO	2.1
1	B	1897	PHE	2.1
1	B	1747	GLY	2.1
1	B	2041	TRP	2.1
1	B	2183	ALA	2.1
1	B	1814	ASN	2.1
1	B	2000	GLY	2.1
1	B	2063	GLY	2.1
1	A	1657	ARG	2.1
1	B	1368	TYR	2.1
1	B	1470	ASN	2.1
1	B	1498	GLU	2.1
1	B	1591	ASP	2.1
1	A	1056	ARG	2.1
1	A	1781	ARG	2.1
1	B	1374	VAL	2.1
1	A	976	MET	2.1
1	B	1757	ARG	2.1
1	B	1932	VAL	2.1
1	A	900	LEU	2.1
1	A	2254	ASP	2.1
1	A	1129	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1582	ILE	2.1
1	B	1562	THR	2.1
1	B	1337	LEU	2.1
1	B	1791	GLY	2.1
1	B	1499	LYS	2.1
1	B	1745	LEU	2.1
1	A	1511	ALA	2.1
1	A	1328	LEU	2.0
1	B	1040	ARG	2.0
1	B	1022	SER	2.0
1	B	1595	LEU	2.0
1	B	1984	GLU	2.0
1	A	2046	PRO	2.0
1	A	1127	TYR	2.0
1	B	1485	PHE	2.0
1	B	1925	LEU	2.0
1	A	2080	LYS	2.0
1	B	1564	ALA	2.0
1	B	1973	THR	2.0
1	A	1432	VAL	2.0
1	A	1097	VAL	2.0
1	B	2075	LYS	2.0
1	A	1843	ILE	2.0
1	B	1956	GLN	2.0
1	B	1879	LYS	2.0
1	A	2185	ASN	2.0
1	B	1638	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.