



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:11 am GMT

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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

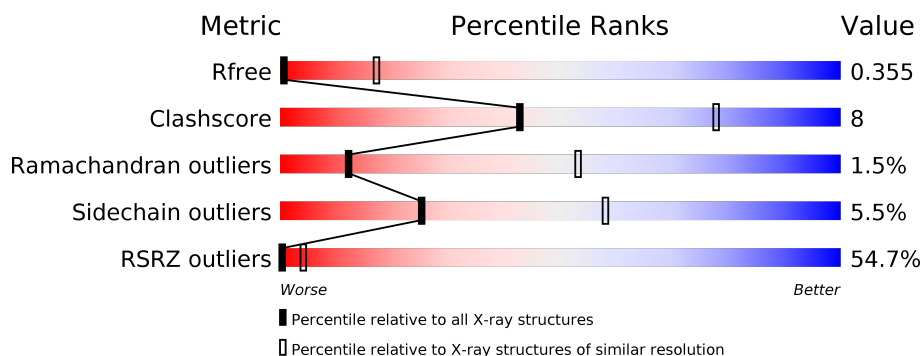
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1100 (10.00-3.70)
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)
RSRZ outliers	101464	1004 (11.50-3.72)

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 $\leq 5\%$. 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			

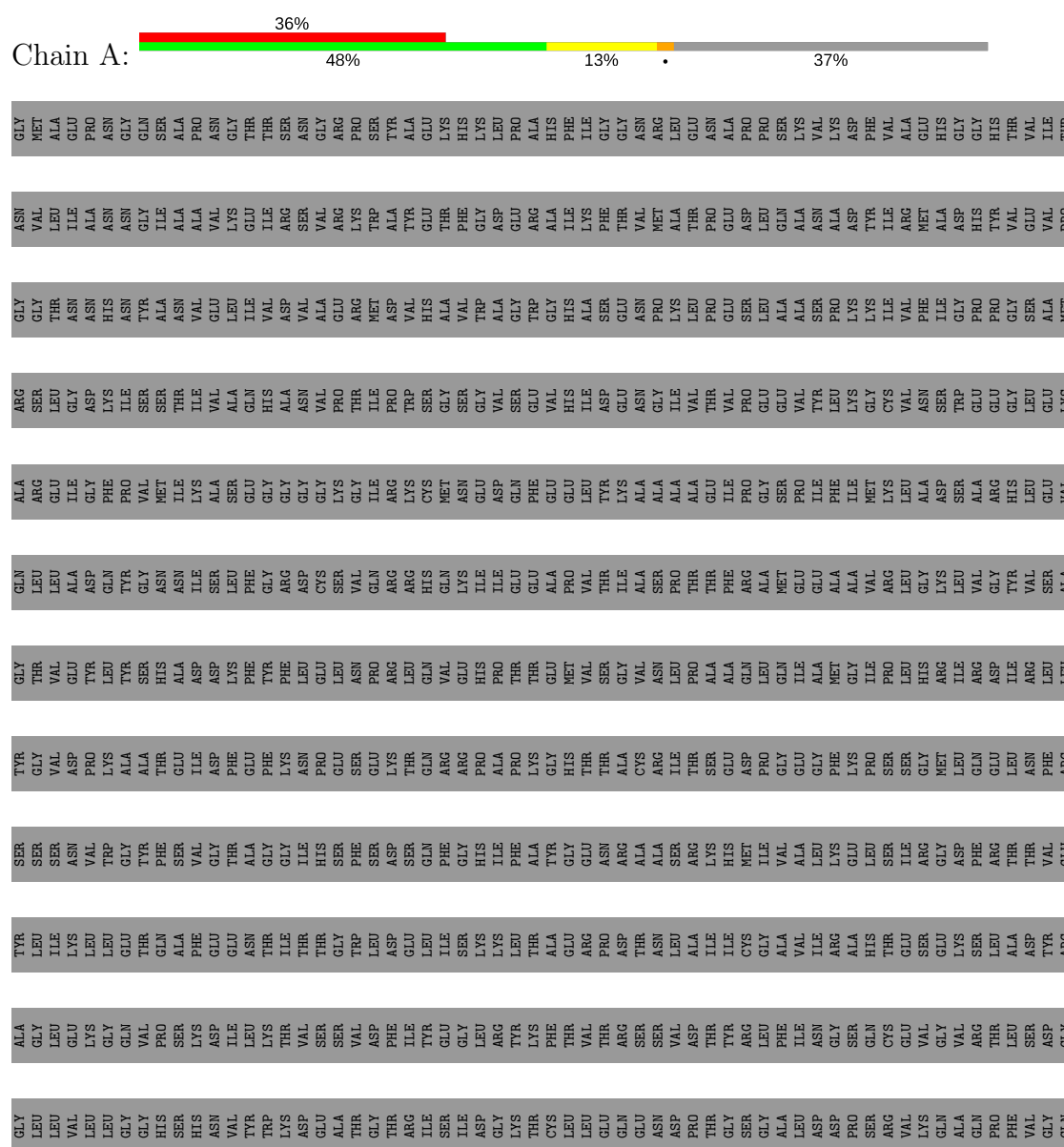
There are 8 discrepancies between the modelled and reference sequences:

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

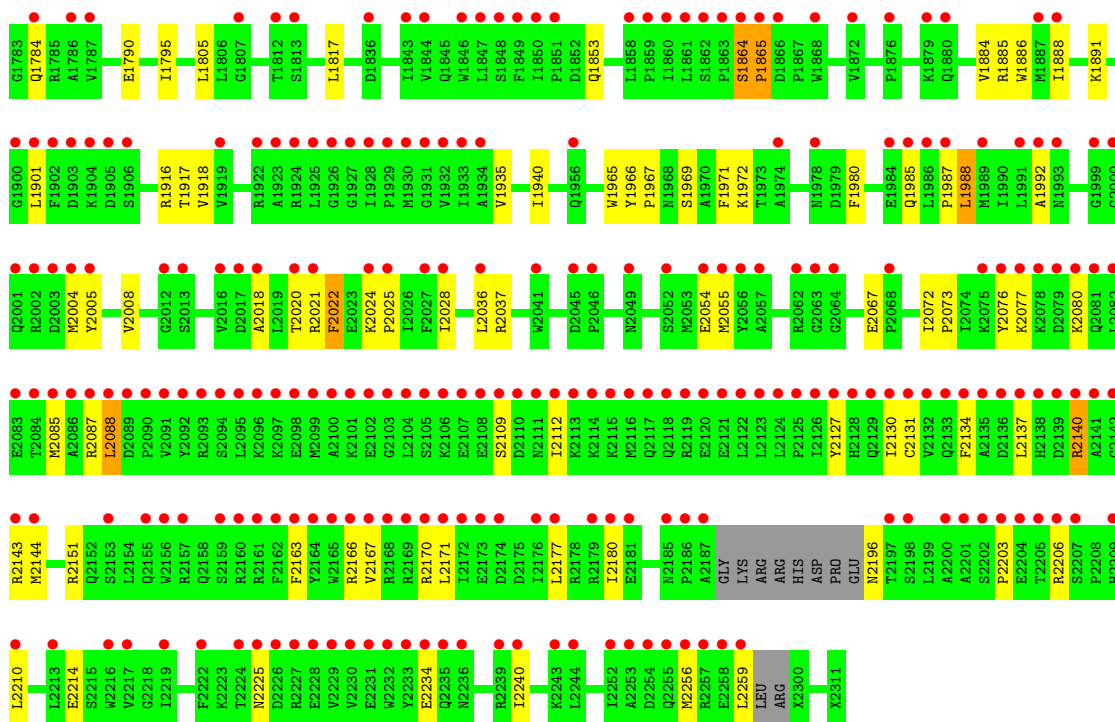
3 Residue-property plots

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

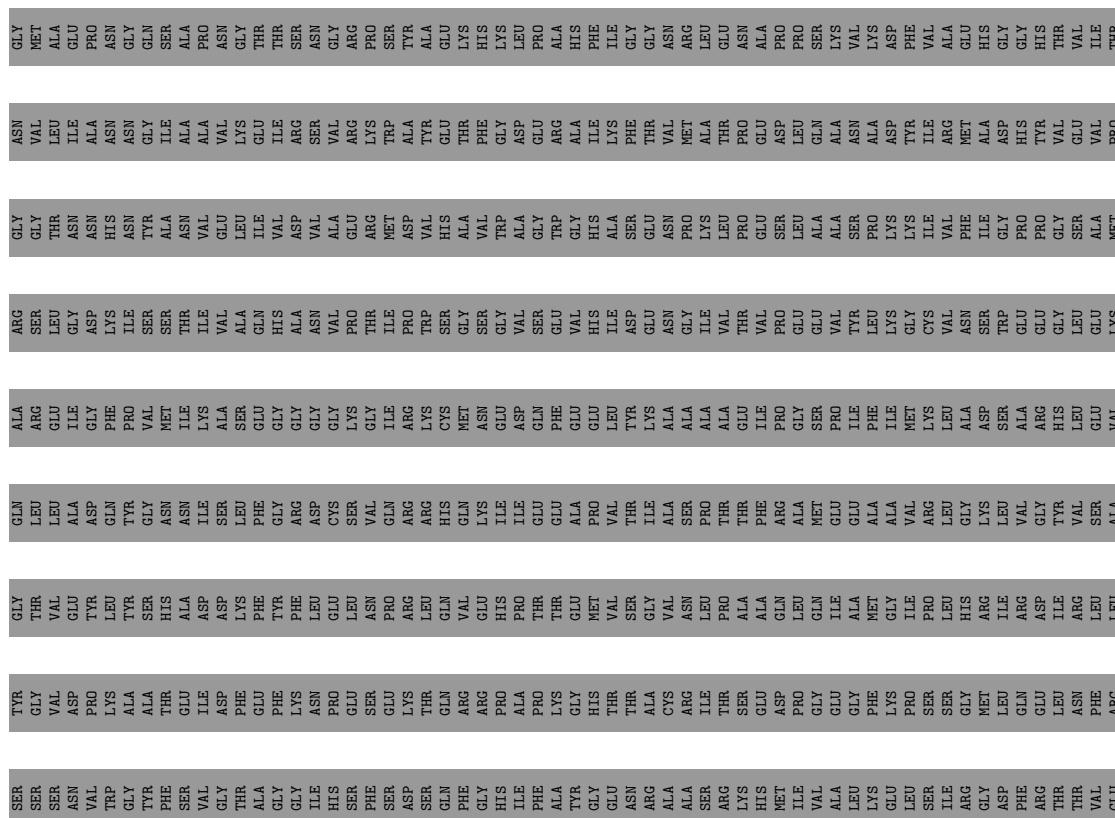
- Molecule 1: Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein



D1705	P1619	V1521	E1431	H1361	R1289	LYS	E1162	Y1096	A1025	V965	L904	R843	LEU
E1706	E1620	S1522	V1432	I1352	V1290	GLN	R1163	Y1097	R1026	V966	E905	Q844	PRO
A1707	T1523	P1524	A1433	H1353	R1291	GLN	A1098	L1098	E1027	N967	P906	GLN	TYR
K1708	P1622	P1524	H1354	V1354	R1292	PRO	F1165	L1099	V1028	T968	L907	S846	GLY
R1709		Y1525	R1451	V1355	L1293	GLY	K1525	A1100	A1100	V969	T908	A847	
R1710		P1526	R1452	E1356	L1294	ILE	R1167	A1101	T1030	L970	S909	L848	S788
F1711		T1527	H1453	R1360	F1295	ALA	I1168	L1102	L1031	S971	V910	H849	P789
		K1528	Q1454	R1361	L1296	ALA	H1169	E1103	CYS	H972	V911	A850	V790
		N1529		L1362	C1297	ASP	V1104	V1104	ALA	R973	N912	R851	V791
				E1363	G1298	LEU	Y1105	Y1105	LEU	N974	L913	M852	V792
				T1364	R1299	ALA	S1172	V1106	PRO	V975	Y914	P853	G793
				D1365	G1302	GLN	M1173	R1107	SER	N976	L915	H854	S794
					S1303	ARG	M1174	R1108	LEU	S977	D916	K855	K795
					Y1304	ARG	T1175	A1109	GLU	K978	G917	L856	P796
					F1305	ARG	Y1176	Y1110	GLU	N979	Q918	D857	Q797
					P1306	PRO	L1177		GLU	S980	K919	A858	A798
					Y1307	THR	A1178	T1041	T1041	L981	A920	K859	R799
					G1308	PRO	R1180	N1114	N1114	V982	R921	L860	F900
					T1309	LEU	T1181	R1115	R1044	L983	E922	T861	A801
					F1310	ARG	R1182	E1117	T1047	A984	L923	Q862	V802
					G1311	LEU	D1183			L986	N924	V863	L803
					G1312	GLU	E1184			L925	L926	L864	Y804
					P1313	GLY	P1185			D987	I926	E865	G805
					Y1315	ILE	I1186			E988	A927	R866	T806
					A1316	GLY	R1187			V989	D928	A867	M807
					E1317	GLU	K1188			R990	L929	Q868	C808
					D1318	LEU	S1055			P991	L930	R869	D809
					F1317	ASP	F1128			N992	M932	G871	L811
					GLU	ASP	T1129			K993	Y933	A872	N812
					ILE	ILE	Y1057			P994	A934	E873	G813
					SER	SER	G1058			V996	D935	F874	Y814
					A1263	A1263	E1059			G997	V936	F875	D815
					V1254	V1255				N998	E937	A876	N816
					V1256	V1257				V999	C938	R877	Q817
					H1322	H1323				G1000	Q939	L878	V818
					I1324	I1325				K1001	F940	R879	V819
					E1326	E1327				H1002	S941	L880	M820
					P1326	P1327				L1003	G942	R891	Q821
					S1327	S1328				R1004	R943	V882	Q822
					L1328	L1329				P1005	R944	F883	K823
					F1330	F1330				V1006	L945	N884	L824
					E1333	E1333				L1007	Q946	K885	K825
					L1334	L1334				D947	D947	F886	K826
					G1335	G1335				R1008	E948	L887	F827
					R1336	R1336				R1009	E949	D888	E828
					L1337	L1337				T1011	A950	D889	E829
					S1338	S1338				E1012	I951	N890	V830
					F1340	F1340				L1013	L952	Y891	L831
					K1341	K1341				E1014	K853	P892	R832
					H1415	H1415				S1015	L954	H893	D833
					H1416	H1416				Q1017	D956	K894	P834
					W1417	W1417				S1018		T895	K835
					F1418	F1418				E1019	K959	P893	L836
					H1423	H1423				K1020	K959	D898	P837
					T1424	T1424				L960	D960	I899	P838
					F1425	F1425				N961	K961	L900	S839
					Q1426	Q1426				L962	L962	K901	E840
					V1427	V1427				S1022	Q963	S902	F841
					T1428	T1428				K1024	K964	T903	S842
					A1429	A1429							
					D1430	D1430							



- 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	462.20Å 462.20Å 204.64Å 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 8.33Å)	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 , 899.5	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	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 [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	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:1081:THR:OG1	1:B:1375:ARG:HB3	2.19	0.43
1:B:1116:ARG:NE	1:B:1132:ASP:HB2	2.31	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:836:LEU:HG	1:A:921:ARG:HH12	1.84	0.42
1:A:831:LEU:HD13	1:A:921:ARG:CZ	2.49	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:831:LEU:HD13	1:B:921:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:LEU:CB	1:B:894:LYS:HE2	2.50	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:1208:LEU:HD21	1:A:1285:LEU:HD23	2.03	0.41
1:A:1275:LYS:HA	1:A:1278:VAL:HG12	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: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:2088:LEU:HG	1:B:1686:VAL:HG23	2.01	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:1794:ILE:HD12	1:B:1823:MET:HG3	2.04	0.40
1:B:993:LYS:HG2	1:B:1031:LEU:HD22	2.03	0.40
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.42	0.40
1:A:2005:TYR:HA	1:B:1826:ASN:HD22	1.87	0.40
1:B:1340:PHE:CZ	1:B:1527:THR:HG22	2.56	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%)	12	53
1	B	1380/2211 (62%)	1249 (90%)	110 (8%)	21 (2%)	12	53
All	All	2753/4422 (62%)	2478 (90%)	233 (8%)	42 (2%)	12	53

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%)	23	56
1	B	1215/1879 (65%)	1151 (95%)	64 (5%)	26	59
All	All	2423/3758 (64%)	2289 (94%)	134 (6%)	25	58

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 4	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 4	5, 230, 485, 500	0

All (1521) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	875	PRO	20.9
1	A	1155	SER	18.6
1	B	874	PHE	18.2
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	2217	VAL	14.0
1	B	1686	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	13.2
1	A	1687	ALA	13.1
1	B	1190	VAL	13.1
1	A	939	GLN	13.0
1	A	1181	THR	12.7
1	A	837	PRO	12.6
1	B	853	PRO	12.4
1	A	842	SER	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	11.6
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	2218	GLY	11.4
1	B	896	ASP	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	791	VAL	11.2
1	B	878	GLN	11.2
1	A	1103	GLU	11.1
1	A	847	ALA	11.1
1	B	1254	VAL	11.1
1	A	1170	SER	11.0
1	B	792	VAL	11.0
1	B	882	VAL	10.9
1	B	1684	PHE	10.9
1	B	1191	ILE	10.9
1	A	1701	LEU	10.9
1	A	2123	LEU	10.9
1	B	892	PRO	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	10.7
1	A	1007	LEU	10.6
1	B	904	LEU	10.6
1	A	1254	VAL	10.6
1	A	1695	GLU	10.5
1	B	1192	VAL	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	10.2
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	927	ALA	9.7
1	A	999	VAL	9.7
1	B	949	GLU	9.7
1	A	1005	PRO	9.7
1	B	2133	GLN	9.7
1	A	790	VAL	9.6
1	B	845	PHE	9.6
1	B	907	LEU	9.5
1	A	1683	HIS	9.5
1	B	1188	LYS	9.5
1	A	857	ASP	9.5
1	A	1029	LEU	9.5
1	A	1730	ILE	9.5
1	A	824	LEU	9.5
1	A	1292	ARG	9.4
1	B	936	VAL	9.4
1	A	1723	ASP	9.4
1	A	986	LEU	9.3
1	B	2132	VAL	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	948	GLU	9.0
1	A	1161	VAL	9.0
1	B	873	GLU	9.0
1	A	833	ASP	9.0
1	B	2134	PHE	9.0
1	A	929	LEU	8.9
1	B	937	GLU	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	B	863	VAL	8.8
1	A	1707	ALA	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	A	2130	ILE	8.6
1	A	2187	ALA	8.6
1	B	834	PRO	8.6
1	B	2197	THR	8.6
1	B	2085	MET	8.6
1	B	2249	LYS	8.6
1	B	876	ALA	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	856	LEU	8.5
1	B	877	ARG	8.5
1	A	1000	GLY	8.5
1	A	858	ALA	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	A	2091	VAL	8.2
1	B	2221	GLY	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	A	968	THR	8.0
1	B	1258	ALA	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	848	LEU	8.0
1	A	949	GLU	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	B	1293	LEU	7.9
1	A	1297	CYS	7.9
1	B	2135	ALA	7.9
1	A	1178	ALA	7.9
1	A	828	ILE	7.9
1	A	850	ALA	7.9
1	B	1169	HIS	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	7.7
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	793	GLY	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	2122	LEU	7.5
1	A	888	ASP	7.5
1	A	1187	ARG	7.5
1	B	883	PHE	7.5
1	B	1106	VAL	7.5
1	B	2128	HIS	7.5
1	B	961	ASN	7.5
1	A	1689	ASN	7.4
1	B	1187	ARG	7.4
1	B	933	TYR	7.4
1	A	1028	VAL	7.4
1	A	1100	ALA	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	B	1732	THR	7.3
1	A	944	ARG	7.3
1	A	855	LYS	7.3
1	B	2125	PRO	7.3
1	A	2102	GLU	7.2
1	A	1703	LEU	7.2
1	A	2138	HIS	7.2
1	B	2232	TRP	7.2
1	B	838	TYR	7.2
1	A	1002	HIS	7.2
1	B	794	SER	7.2
1	A	1058	GLY	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	921	ARG	7.1
1	B	1619	PRO	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	6.8
1	A	1156	SER	6.8
1	B	1153	VAL	6.8
1	A	2086	ALA	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	B	2017	ASP	6.7
1	A	1010	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	2104	LEU	6.7
1	A	2173	GLU	6.7
1	A	934	ALA	6.6
1	A	1153	VAL	6.6
1	A	1160	PRO	6.6
1	A	883	PHE	6.6
1	A	1162	GLU	6.6
1	A	979	ASN	6.6
1	B	2230	VAL	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	A	1727	ARG	6.5
1	B	1200	ALA	6.5
1	B	888	ASP	6.5
1	B	1695	GLU	6.5
1	A	1180	ARG	6.5
1	A	2111	ASN	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	A	1295	PHE	6.4
1	B	2214	GLU	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	A	1025	ALA	6.2
1	B	2165	TRP	6.2
1	B	951	ILE	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	A	2167	VAL	6.1
1	B	799	ARG	6.1
1	A	1018	SER	6.1
1	A	1193	PRO	6.1
1	B	2204	GLU	6.1
1	A	2096	LYS	6.1
1	A	2105	SER	6.1
1	A	2163	PHE	6.0
1	A	1574	LYS	6.0
1	B	2020	THR	6.0
1	B	1424	THR	6.0
1	A	923	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	865	GLU	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	912	ASN	6.0
1	A	1307	TYR	6.0
1	B	2120	GLU	6.0
1	A	1154	PRO	6.0
1	A	952	LEU	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	A	969	VAL	5.9
1	B	1678	GLU	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	955	ARG	5.8
1	A	1717	THR	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	1011	THR	5.8
1	A	2000	GLY	5.8
1	B	1728	HIS	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	B	832	ARG	5.7
1	B	974	ASN	5.7
1	A	2108	GLU	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	B	985	LEU	5.7
1	B	2256	MET	5.7
1	A	886	PHE	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	B	1618	THR	5.6
1	B	2081	GLN	5.6
1	A	967	ASN	5.6
1	A	1312	GLY	5.6
1	A	1715	VAL	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	A	2165	TRP	5.5
1	B	957	GLN	5.5
1	B	2261	ARG	5.5
1	B	818	VAL	5.5
1	B	2247	LEU	5.5
1	B	1160	PRO	5.5
1	B	1179	ARG	5.5
1	B	2155	GLN	5.5
1	A	1020	LYS	5.5
1	B	1459	ILE	5.5
1	A	1012	GLU	5.5
1	A	2170	ARG	5.4
1	B	1291	ARG	5.4
1	A	1706	GLU	5.4
1	A	2216	TRP	5.4
1	B	1104	VAL	5.4
1	B	2157	ARG	5.4
1	A	1044	MET	5.4
1	B	1729	LYS	5.4
1	A	2159	SER	5.4
1	A	910	VAL	5.4
1	A	998	ASN	5.4
1	B	1208	LEU	5.4
1	B	867	ALA	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	A	2232	TRP	5.4
1	B	922	GLU	5.4
1	B	2244	LEU	5.4
1	A	1476	ARG	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	1021	VAL	5.3
1	A	1289	ARG	5.3
1	B	1167	ARG	5.3
1	A	1285	LEU	5.3
1	A	1864	SER	5.3
1	A	2135	ALA	5.3
1	A	825	LYS	5.3
1	A	830	VAL	5.3
1	A	863	VAL	5.3
1	A	1363	GLU	5.3
1	B	971	SER	5.3
1	B	982	VAL	5.3
1	A	931	SER	5.3
1	B	1133	PHE	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	B	859	GLN	5.2
1	A	1294	THR	5.2
1	B	1760	ASN	5.2
1	B	1119	ARG	5.2
1	A	800	PHE	5.2
1	A	928	ASP	5.2
1	A	1354	VAL	5.2
1	A	2018	ALA	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	B	1865	PRO	5.1
1	A	1353	HIS	5.1
1	A	2113	LYS	5.1
1	A	1756	SER	5.1
1	B	935	ASP	5.1
1	A	1734	VAL	5.1
1	B	930	LEU	5.1
1	B	1170	SER	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	2021	ARG	5.0
1	B	2156	TRP	5.0
1	A	1057	TYR	5.0
1	A	1620	GLU	5.0
1	B	1795	ILE	5.0
1	B	891	VAL	5.0
1	B	2231	GLU	5.0
1	B	890	ASN	5.0
1	B	1207	ALA	5.0
1	B	1018	SER	5.0
1	A	1258	ALA	5.0
1	A	1729	LYS	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	A	1987	PRO	4.9
1	B	2174	ASP	4.9
1	B	926	ILE	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	A	1726	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1475	LEU	4.8
1	B	1292	ARG	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	A	2056	TYR	4.8
1	B	827	PHE	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	1109	ALA	4.8
1	B	2013	SER	4.8
1	A	2107	GLU	4.8
1	B	966	VAL	4.8
1	B	978	LYS	4.8
1	A	1733	ILE	4.8
1	B	988	GLU	4.7
1	B	938	CYS	4.7
1	A	1182	ARG	4.7
1	A	954	LEU	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	1199	ASP	4.7
1	B	880	LEU	4.7
1	A	1696	ALA	4.7
1	B	1734	VAL	4.7
1	A	815	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	897	GLN	4.7
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	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	850	ALA	4.6
1	B	1872	VAL	4.6
1	B	2086	ALA	4.6
1	B	887	LEU	4.6
1	B	2167	VAL	4.6
1	A	2169	ARG	4.6
1	A	1521	VAL	4.6
1	A	894	LYS	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	877	ARG	4.6
1	A	922	GLU	4.6
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	B	1978	ASN	4.5
1	A	935	ASP	4.5
1	B	956	ASP	4.5
1	A	1027	GLU	4.5
1	B	2162	PHE	4.5
1	B	2255	GLN	4.5
1	B	1426	GLN	4.5
1	A	2100	ALA	4.5
1	B	1981	ASN	4.4
1	B	1863	PRO	4.4
1	A	1862	SER	4.4
1	B	1477	VAL	4.4
1	A	918	GLN	4.4
1	A	1083	PHE	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	B	1705	ASP	4.3
1	A	2076	TYR	4.3
1	A	2106	LYS	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	A	1760	ASN	4.3
1	B	1861	LEU	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	2158	GLN	4.3
1	B	2049	ASN	4.3
1	A	1926	GLY	4.3
1	A	1848	SER	4.3
1	A	826	GLU	4.3
1	A	904	LEU	4.3
1	A	1373	VAL	4.3
1	B	1575	GLN	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	A	2257	ARG	4.2
1	B	1691	PRO	4.2
1	B	1124	GLU	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	B	1206	ARG	4.2
1	A	971	SER	4.2
1	A	2197	THR	4.2
1	B	1603	GLY	4.2
1	A	832	ARG	4.1
1	B	929	LEU	4.1
1	B	1719	GLU	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	1429	ALA	4.1
1	B	1693	LYS	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	A	1324	ILE	4.0
1	A	1865	PRO	4.0
1	B	2254	ASP	4.0
1	A	1522	SER	4.0
1	B	1210	VAL	4.0
1	B	981	LEU	4.0
1	A	1708	LYS	4.0
1	A	1311	ARG	4.0
1	B	1297	CYS	4.0
1	B	1161	VAL	4.0
1	A	1880	GLN	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	902	SER	4.0
1	B	2023	GLU	4.0
1	B	1158	ALA	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	3.9
1	B	828	ILE	3.9
1	A	1298	GLY	3.9
1	A	1211	LEU	3.9
1	A	1622	PRO	3.9
1	B	975	VAL	3.9
1	A	909	SER	3.9
1	B	953	LYS	3.9
1	A	2137	LEU	3.9
1	B	1120	TYR	3.9
1	A	1069	ARG	3.9
1	B	1735	GLY	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	2140	ARG	3.9
1	A	932	MET	3.9
1	A	2222	PHE	3.9
1	A	2110	ASP	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	A	2177	LEU	3.8
1	A	2180	ILE	3.8
1	B	960	ASP	3.8
1	A	797	ALA	3.8
1	A	867	ALA	3.8
1	A	2160	ARG	3.8
1	B	905	GLU	3.8
1	B	1949	ALA	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	1013	LEU	3.8
1	B	1979	ASP	3.8
1	A	2258	GLU	3.8
1	B	1092	HIS	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	A	1174	MET	3.8
1	B	1308	TYR	3.8
1	A	1502	TRP	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	A	2141	ALA	3.7
1	B	1017	GLN	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	A	2236	ASN	3.7
1	B	1868	TRP	3.7
1	B	2118	GLN	3.7
1	B	811	LEU	3.7
1	A	1858	LEU	3.7
1	A	966	VAL	3.7
1	A	811	LEU	3.7
1	B	861	THR	3.7
1	B	1761	ASP	3.7
1	A	788	SER	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	A	1364	THR	3.6
1	A	2213	LEU	3.6
1	B	954	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	1862	SER	3.6
1	B	2251	SER	3.6
1	A	1048	LEU	3.6
1	B	1724	GLY	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	2121	GLU	3.6
1	B	2209	HIS	3.6
1	B	2198	SER	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	A	1989	MET	3.5
1	B	1560	SER	3.5
1	B	2025	PRO	3.5
1	A	1347	THR	3.5
1	B	1588	VAL	3.5
1	A	1849	PHE	3.5
1	B	1121	HIS	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	1492	TYR	3.4
1	A	2171	LEU	3.4
1	B	801	ALA	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	2062	ARG	3.3
1	A	2172	ILE	3.3
1	B	854	HIS	3.3
1	A	898	ASP	3.3
1	A	2228	GLU	3.3
1	B	1866	ASP	3.3
1	B	1718	GLU	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	A	2128	HIS	3.3
1	B	2054	GLU	3.3
1	B	1627	PHE	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	1931	GLY	3.3
1	A	1410	ASN	3.3
1	B	2069	GLU	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	B	2142	GLY	3.2
1	B	2022	PHE	3.2
1	A	1482	THR	3.2
1	B	1598	VAL	3.2
1	A	1274	ILE	3.2
1	B	947	ASP	3.2
1	A	1375	ARG	3.2
1	B	1576	PRO	3.2
1	A	1345	VAL	3.2
1	B	1010	LEU	3.2
1	A	2209	HIS	3.2
1	B	1159	THR	3.2
1	A	1495	LYS	3.2
1	A	1678	GLU	3.2
1	B	1721	VAL	3.2
1	B	2065	VAL	3.2
1	A	961	ASN	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	A	1543	THR	3.2
1	B	946	GLN	3.2
1	A	2244	LEU	3.2
1	B	1491	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	870	ARG	3.2
1	B	2186	PRO	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	915	LEU	3.1
1	A	1932	VAL	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	B	2160	ARG	3.1
1	A	2179	ARG	3.1
1	B	2207	SER	3.1
1	A	2240	ILE	3.1
1	A	1637	LYS	3.1
1	B	1427	VAL	3.1
1	B	1682	PRO	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	A	1518	LEU	3.1
1	B	1711	PHE	3.1
1	A	975	VAL	3.1
1	B	871	GLY	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	1374	VAL	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	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	1471	ASP	3.0
1	B	942	GLY	3.0
1	B	1156	SER	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	B	866	ARG	3.0
1	B	1637	LYS	3.0
1	A	1562	THR	3.0
1	B	1710	ARG	3.0
1	B	2019	LEU	3.0
1	A	1370	THR	2.9
1	A	2129	GLN	2.9
1	B	1987	PRO	2.9
1	B	1982	TYR	2.9
1	A	1710	ARG	2.9
1	B	958	TYR	2.9
1	B	1326	PRO	2.9
1	A	1204	LEU	2.9
1	A	1544	GLN	2.9
1	B	1706	GLU	2.9
1	B	1336	ARG	2.9
1	A	1075	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1300	ASN	2.9
1	B	2241	ASN	2.9
1	A	901	LYS	2.9
1	A	2227	ARG	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	A	1985	GLN	2.9
1	B	1867	PRO	2.9
1	B	962	ILE	2.9
1	B	1454	GLN	2.9
1	A	2005	TYR	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	866	ARG	2.9
1	A	1081	THR	2.8
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	B	1421	PHE	2.8
1	B	2171	LEU	2.8
1	A	1425	PHE	2.8
1	A	2136	ASP	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	B	1209	GLU	2.8
1	A	1117	GLU	2.8
1	B	1181	THR	2.8
1	B	1338	SER	2.8
1	A	2016	VAL	2.8
1	B	2179	ARG	2.8
1	B	1478	ILE	2.8
1	B	2032	PRO	2.8
1	A	1846	TRP	2.8
1	B	1561	TRP	2.7
1	B	1928	ILE	2.7
1	B	1356	GLU	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	A	1627	PHE	2.7
1	B	1586	GLU	2.7
1	A	1709	ARG	2.7
1	A	1887	MET	2.7
1	A	2049	ASN	2.7
1	A	870	ARG	2.7
1	A	1208	LEU	2.7
1	A	1617	ARG	2.7
1	A	1625	ARG	2.7
1	B	1128	PHE	2.7
1	A	1079	LYS	2.7
1	B	1116	ARG	2.7
1	A	2078	LYS	2.7
1	A	814	TYR	2.7
1	A	1546	VAL	2.7
1	B	1628	ILE	2.7
1	A	919	LYS	2.7
1	A	2079	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1888	ILE	2.7
1	A	2153	SER	2.7
1	A	1133	PHE	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	1420	ASN	2.6
1	B	1989	MET	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	B	1600	ARG	2.6
1	A	871	GLY	2.6
1	B	1888	ILE	2.6
1	A	1571	LEU	2.6
1	A	1157	PRO	2.6
1	A	1371	ARG	2.6
1	B	1044	MET	2.6
1	A	1344	PRO	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	A	1379	LEU	2.5
1	B	1112	ALA	2.5
1	B	1736	ALA	2.5
1	B	1786	ALA	2.5
1	A	2012	GLY	2.5
1	B	1697	GLY	2.5
1	B	1457	ILE	2.5
1	A	1524	PRO	2.5
1	A	903	THR	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	1926	GLY	2.5
1	B	1930	MET	2.5
1	A	1812	THR	2.5
1	B	2083	GLU	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	2161	ARG	2.5
1	B	1355	TYR	2.4
1	A	1321	ILE	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	B	934	ALA	2.4
1	B	1378	ARG	2.4
1	A	1404	LEU	2.4
1	A	2055	MET	2.4
1	B	798	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	819	VAL	2.4
1	B	915	LEU	2.4
1	A	2201	ALA	2.4
1	B	1573	ALA	2.4
1	B	1934	ALA	2.4
1	A	1787	VAL	2.4
1	B	826	GLU	2.4
1	B	1545	TYR	2.4
1	B	1115	LEU	2.4
1	B	994	PRO	2.4
1	A	2231	GLU	2.4
1	A	1055	SER	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	A	1326	PRO	2.4
1	A	819	VAL	2.4
1	A	1844	VAL	2.4
1	A	2234	GLU	2.4
1	B	1462	MET	2.4
1	A	1592	GLN	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	1315	TYR	2.3
1	B	1898	GLN	2.3
1	B	1003	LEU	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	1599	SER	2.3
1	A	1784	GLN	2.3
1	A	1876	PRO	2.3
1	B	1525	TYR	2.3
1	A	2077	LYS	2.3
1	B	2014	PHE	2.3
1	A	1594	ASN	2.3
1	A	1993	ASN	2.3
1	A	1078	SER	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	1919	VAL	2.3
1	B	1844	VAL	2.3
1	A	1049	ARG	2.3
1	A	1319	ASP	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	B	1996	GLY	2.2
1	A	1872	VAL	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	1927	GLY	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	A	1956	GLN	2.2
1	B	1593	ASP	2.2
1	B	1753	GLY	2.2
1	B	1746	ARG	2.2
1	A	1426	GLN	2.2
1	B	987	ASP	2.2
1	B	1764	THR	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	1545	TYR	2.1
1	A	1610	VAL	2.1
1	A	1302	GLY	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	1157	PRO	2.1
1	B	1897	PHE	2.1
1	B	1317	GLU	2.1
1	B	1747	GLY	2.1
1	B	2063	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	1368	TYR	2.1
1	A	1657	ARG	2.1
1	B	1470	ASN	2.1
1	B	1498	GLU	2.1
1	A	1056	ARG	2.1
1	A	1781	ARG	2.1
1	B	1591	ASP	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	1791	GLY	2.1
1	B	1337	LEU	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	1925	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	1564	ALA	2.0
1	A	2080	LYS	2.0
1	A	1432	VAL	2.0
1	A	1097	VAL	2.0
1	B	1973	THR	2.0
1	B	2075	LYS	2.0
1	A	1843	ILE	2.0
1	B	1638	ILE	2.0
1	B	1956	GLN	2.0
1	B	1879	LYS	2.0
1	A	2185	ASN	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.