



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:16 AM EDT

PDB ID : 6TS8  
Title : Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) double cysteine mutant G177C/A786C.  
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Deposited on : 2019-12-20  
Resolution : 4.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

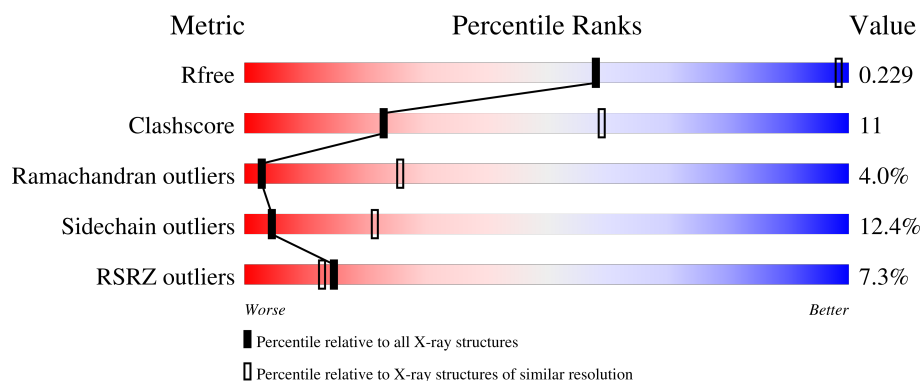
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1382	<div> <div>5%</div> <div>58%</div> <div>28%</div> <div>9%</div> </div>
1	B	1382	<div> <div>9%</div> <div>58%</div> <div>28%</div> <div>9%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20112 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 UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1254	Total	C	N	O	S	0	0	0
			10056	6439	1711	1879	27			
1	B	1254	Total	C	N	O	S	0	0	0
			10056	6439	1711	1879	27			

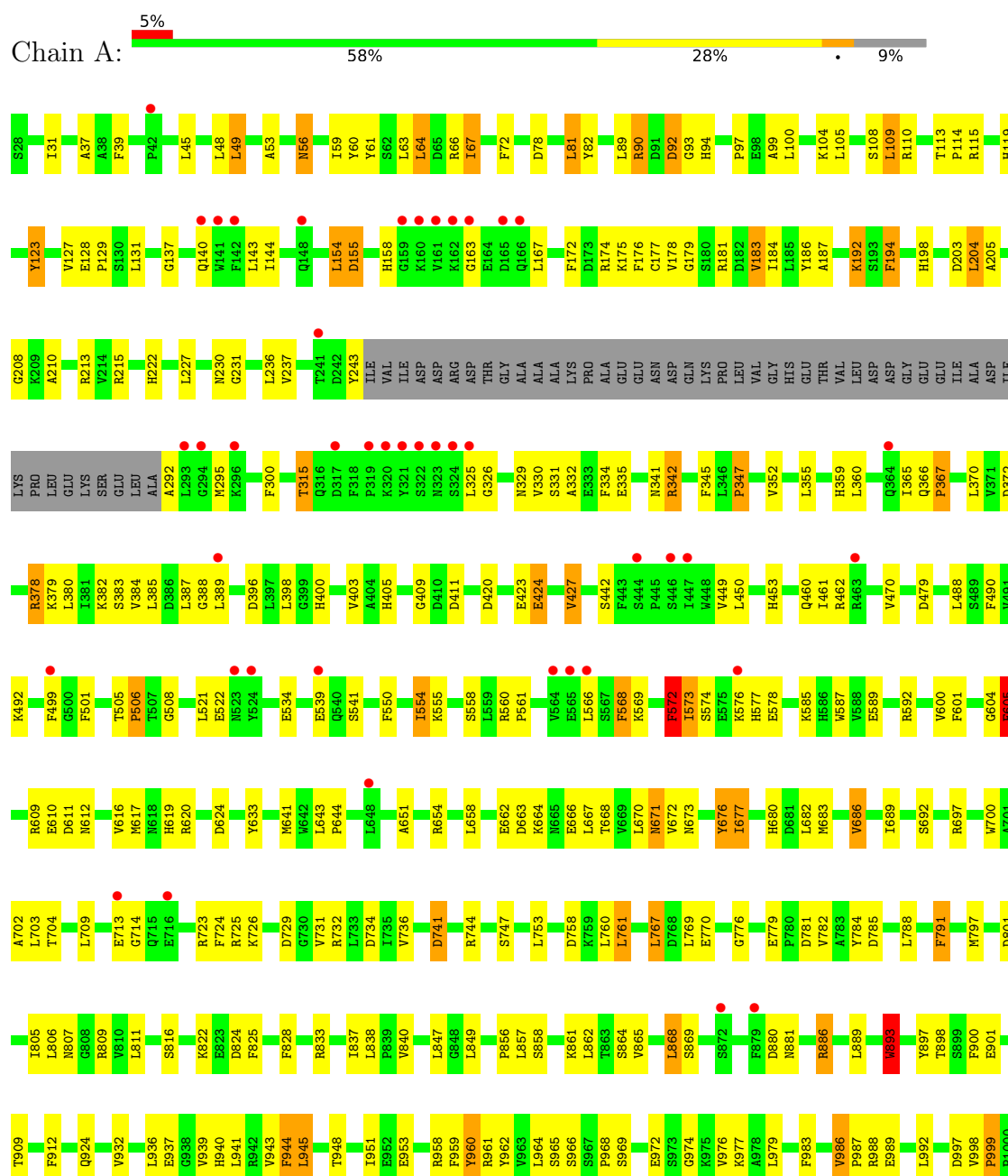
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	CYS	GLY	engineered mutation	UNP G0SB58
A	786	CYS	ALA	engineered mutation	UNP G0SB58
B	177	CYS	GLY	engineered mutation	UNP G0SB58
B	786	CYS	ALA	engineered mutation	UNP G0SB58

### 3 Residue-property plots [i](#)

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

- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein





THR	GLY	TYR	ALA	ASN	TYR	LEU	LYS	LYS	PRO	TYR	HIS	ILE	SER	ALA	L1361	Y1362	Y1363	V1364	D1365	L1366	Y1369	D1376	R1377	L1378	Q1381	S1391	L1392	A1393	N1394	L1395	D1398	L1399	P1400	N1401	H1402	H1403	T1406	I1407	P1408	I1409																	
W1265	P1266	L1269	R1270	Q1271	Q1272	E1278	S1204	W1279	W1280	G1281	K1282	K1283	F1286	L1287	D1288	V1289	L1290	F1291	D1296	K1297	F1300	I1306	V1307	R1308	T1309	D1310	M1311	Y1312	D1313	L1314	V1315	A1322	P1323	Y1324	GLY	PHE	ALA	PRO	MET	CYS	ASP	SER	ARG	VAL	GLU	MET	GLY	TYR	GLY	ARG	PHE	TRP	LYS				
THR	GLY	THR	ALA	ASN	TYR	LEU	LYS	LYS	PRO	TYR	HIS	ILE	SER	ALA	L1211	M1214	L1215	L1216	L1217	M1218	M1219	A1220	S1221	V1222	M1223	H1224	H1225	T1226	M1227	H1228	T1229	V1230	K1231	F1232	W1233	F1234	I1235	E1236	Q1237	F1238	L1239	S1240	P1241	K1244	D1245	F1246	H1249	M1250	Y1254	G1255	F1256	K1257	Y1258	E1259	M1261	V1262	LYS
F1129	Q1130	T1132	T1133	L1134	Y1135	P1136	R1137	L1138	E1146	E1147	D1148	V1149	L1150	E1151	P1152	SER	THR	LYS	SER	GLY	GLU	GLY	SER	GLY	GLY	ASN	ASN	LEU	VAL	SER	ARG	GLY	ILE	LYS	PHE	ALA	GLU	GLY	LEU	LEU	GLY	ARG	GLY	ASN	LYS	ALA	ALA	GLU	GLY	ALA	THR	LYS	SER	VAL	LYS		
I1041	S1045	R1046	E1047	I1048	P1049	G1050	P1054	R1055	P1056	Q1058	V1059	G1060	P1067	H1068	D1071	L1072	I1073	Y1080	F1081	Q1082	F1083	R1084	A1085	V1088	R1093	L1094	G1097	R1098	S1099	I1102	F1103	T1104	L1105	E1106	S1107	V1108	G1109	P1115	I1116	G1118	D1119	D1120	N1121	T1122	M1127	D1128	LYS										
R958	F959	Y960	R961	Y962	Y963	L964	S965	S966	P967	P968	S969	E972	S973	G974	K975	Y976	K977	A978	L979	S980	F983	Y986	P987	R988	E989	L992	Y996	D997	Y998	P999	F1000	A1001	W1002	L1003	V1008	D1011	D1012	L1016	R1017	I1018	V1030	E1031	A1032	I1033	Y1034	E1037	H1038	T1039	L1040	K957							
T668	F669	L670	N671	V672	N673	Y676	L677	H680	L682	M683	D684	L685	V686	L689	S692	R697	W700	A701	A702	L703	T704	L709	E713	G714	Q715	R723	F724	R725	K726	D729	G730	V731	R732	L733	D734	I735	V736	D741	R744	S747	L753	D758	K759	L760													
L761	D767	L768	E770	G776	E777	L778	E779	D780	V781	V782	A783	D785	L788	F791	M797	D801	I805	L806	F900	N807	G808	V809	V810	L811	S816	K822	E823	D824	F825	L828	H833	I837	L838	R839	Y840	L847	G848	L849	P856	L857	S858	K861	L862														

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.05Å 139.05Å 176.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	139.04 – 4.60 139.05 – 4.77	Depositor EDS
% Data completeness (in resolution range)	32.1 (139.04-4.60) 36.0 (139.05-4.77)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 4.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.203 , 0.234 0.202 , 0.229	Depositor DCC
$R_{free}$ test set	339 reflections (5.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	206.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 500.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	20112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [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	0.64	0/10293	0.77	0/13959
1	B	0.63	0/10293	0.76	0/13959
All	All	0.63	0/20586	0.76	0/27918

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	10056	0	9955	226	0
1	B	10056	0	9955	231	0
All	All	20112	0	19910	457	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 11.

All (457) 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:1109:GLY:H	1:A:1136:PRO:HA	1.12	1.11
1:B:1109:GLY:H	1:B:1136:PRO:HA	1.12	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:HA	1:A:385:LEU:HG	1.51	0.93
1:B:382:LYS:HA	1:B:385:LEU:HG	1.51	0.92
1:B:833:ARG:HA	1:B:837:ILE:HB	1.55	0.87
1:A:833:ARG:HA	1:A:837:ILE:HB	1.55	0.85
1:B:704:THR:HB	1:B:805:ILE:HB	1.59	0.85
1:A:704:THR:HB	1:A:805:ILE:HB	1.59	0.84
1:A:123:TYR:HA	1:A:127:VAL:HB	1.60	0.83
1:B:345:PHE:HB3	1:B:893:TRP:NE1	1.94	0.82
1:A:345:PHE:HB3	1:A:893:TRP:NE1	1.95	0.82
1:A:342:ARG:HG2	1:A:347:PRO:HA	1.63	0.81
1:B:123:TYR:HA	1:B:127:VAL:HB	1.60	0.81
1:B:342:ARG:HG2	1:B:347:PRO:HA	1.64	0.80
1:A:901:GLU:OE1	1:A:940:HIS:NE2	2.16	0.78
1:A:676:TYR:HA	1:A:683:MET:HG3	1.68	0.75
1:B:676:TYR:HA	1:B:683:MET:HG3	1.67	0.75
1:A:932:VAL:HG21	1:A:964:LEU:HB3	1.69	0.74
1:B:932:VAL:HG21	1:B:964:LEU:HB3	1.69	0.73
1:A:671:ASN:HA	1:A:864:SER:HB3	1.72	0.72
1:B:1109:GLY:N	1:B:1136:PRO:HA	1.97	0.72
1:A:31:ILE:HA	1:A:1030:VAL:HB	1.72	0.72
1:A:1109:GLY:N	1:A:1136:PRO:HA	1.97	0.71
1:B:671:ASN:HA	1:B:864:SER:HB3	1.71	0.71
1:B:384:VAL:HA	1:B:387:LEU:HG	1.73	0.71
1:B:901:GLU:OE1	1:B:940:HIS:NE2	2.16	0.70
1:A:61:TYR:OH	1:A:174:ARG:O	2.08	0.70
1:B:61:TYR:OH	1:B:174:ARG:O	2.08	0.70
1:A:384:VAL:HA	1:A:387:LEU:HG	1.73	0.70
1:B:31:ILE:HA	1:B:1030:VAL:HB	1.73	0.70
1:B:115:ARG:HA	1:B:1127:MET:HB2	1.73	0.69
1:A:342:ARG:CG	1:A:347:PRO:HA	2.23	0.69
1:A:115:ARG:HA	1:A:1127:MET:HB2	1.75	0.68
1:B:64:LEU:HD23	1:B:198:HIS:CE1	2.29	0.68
1:A:64:LEU:HD23	1:A:198:HIS:CE1	2.28	0.67
1:B:342:ARG:CG	1:B:347:PRO:HA	2.23	0.67
1:B:1201:ASN:HB3	1:B:1233:TRP:HE1	1.59	0.67
1:A:1201:ASN:HB3	1:A:1233:TRP:HE1	1.60	0.66
1:B:898:THR:HB	1:B:945:LEU:HB3	1.78	0.66
1:B:1225:HIS:CD2	1:B:1308:ARG:HA	2.30	0.66
1:B:1109:GLY:H	1:B:1136:PRO:CA	2.01	0.66
1:A:898:THR:HB	1:A:945:LEU:HB3	1.78	0.66
1:A:988:ARG:HA	1:A:1018:ILE:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:ARG:HA	1:B:1018:ILE:HB	1.78	0.65
1:A:1225:HIS:CD2	1:A:1308:ARG:HA	2.31	0.65
1:B:658:LEU:HB3	1:B:811:LEU:HB3	1.79	0.65
1:A:236:LEU:HB3	1:A:992:LEU:HB3	1.79	0.65
1:A:78:ASP:HB2	1:A:974:GLY:O	1.97	0.65
1:A:398:LEU:HB3	1:A:886:ARG:HD3	1.79	0.65
1:B:236:LEU:HB3	1:B:992:LEU:HB3	1.79	0.64
1:B:378:ARG:HE	1:B:909:THR:HG21	1.62	0.64
1:A:378:ARG:HE	1:A:909:THR:HG21	1.61	0.64
1:B:78:ASP:HB2	1:B:974:GLY:O	1.97	0.64
1:B:105:LEU:HD12	1:B:966:SER:HA	1.79	0.64
1:B:398:LEU:HB3	1:B:886:ARG:HD3	1.79	0.64
1:A:658:LEU:HB3	1:A:811:LEU:HB3	1.79	0.64
1:A:858:SER:O	1:A:862:LEU:HG	1.98	0.64
1:B:858:SER:O	1:B:862:LEU:HG	1.98	0.63
1:A:105:LEU:HD12	1:A:966:SER:HA	1.79	0.63
1:A:192:LYS:HE2	1:A:192:LYS:HA	1.81	0.62
1:A:411:ASP:HA	1:A:664:LYS:HB3	1.80	0.62
1:B:411:ASP:HA	1:B:664:LYS:HB3	1.80	0.62
1:B:1311:MET:HA	1:B:1314:LEU:HD13	1.81	0.61
1:B:192:LYS:HA	1:B:192:LYS:HE2	1.81	0.61
1:A:1311:MET:HA	1:A:1314:LEU:HD13	1.83	0.61
1:B:140:GLN:HG3	1:B:187:ALA:HA	1.83	0.61
1:A:341:ASN:O	1:A:893:TRP:NE1	2.33	0.60
1:A:1109:GLY:H	1:A:1136:PRO:CA	2.01	0.60
1:B:341:ASN:O	1:B:893:TRP:NE1	2.33	0.60
1:A:686:VAL:HG11	1:A:736:VAL:HG22	1.84	0.60
1:A:237:VAL:O	1:A:992:LEU:HA	2.02	0.60
1:A:352:VAL:HG13	1:A:359:HIS:HD2	1.67	0.59
1:A:689:ILE:HG21	1:A:761:LEU:HD21	1.85	0.59
1:B:366:GLN:HB2	1:B:367:PRO:HD2	1.83	0.59
1:B:1322:ALA:HA	1:B:1408:PRO:HB2	1.85	0.59
1:B:686:VAL:HG11	1:B:736:VAL:HG22	1.84	0.59
1:A:56:ASN:HB3	1:A:59:ILE:HB	1.83	0.59
1:A:140:GLN:HG3	1:A:187:ALA:HA	1.83	0.59
1:B:689:ILE:HG21	1:B:761:LEU:HD21	1.85	0.59
1:A:366:GLN:HB2	1:A:367:PRO:HD2	1.84	0.59
1:B:237:VAL:O	1:B:992:LEU:HA	2.02	0.58
1:B:352:VAL:HG13	1:B:359:HIS:HD2	1.68	0.58
1:B:1205:VAL:HG11	1:B:1283:LYS:HE2	1.85	0.58
1:A:450:LEU:HD11	1:A:461:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HB2	1:A:959:PHE:HB2	1.86	0.58
1:A:1322:ALA:HA	1:A:1408:PRO:HB2	1.84	0.58
1:B:833:ARG:HG3	1:B:838:LEU:HG	1.86	0.58
1:A:676:TYR:OH	1:A:704:THR:OG1	2.18	0.58
1:B:1039:ILE:O	1:B:1085:ALA:O	2.22	0.57
1:B:236:LEU:HB2	1:B:959:PHE:HB2	1.86	0.57
1:A:1039:ILE:O	1:A:1085:ALA:O	2.21	0.57
1:B:450:LEU:HD11	1:B:461:ILE:HD13	1.87	0.57
1:A:411:ASP:HA	1:A:664:LYS:CB	2.35	0.57
1:B:179:GLY:HA3	1:B:210:ALA:HA	1.86	0.57
1:B:360:LEU:HB2	1:B:365:ILE:HD11	1.87	0.57
1:B:725:ARG:HD3	1:B:731:VAL:HB	1.86	0.57
1:A:179:GLY:HA3	1:A:210:ALA:HA	1.86	0.57
1:B:411:ASP:HA	1:B:664:LYS:CB	2.35	0.57
1:A:1223:MET:HG3	1:A:1256:PHE:HB3	1.87	0.57
1:A:725:ARG:HD3	1:A:731:VAL:HB	1.86	0.56
1:B:56:ASN:HB3	1:B:59:ILE:HB	1.85	0.56
1:B:1296:ASP:HA	1:B:1366:LEU:HB2	1.88	0.56
1:B:1108:VAL:HA	1:B:1136:PRO:HB3	1.87	0.56
1:A:360:LEU:HB2	1:A:365:ILE:HD11	1.87	0.56
1:A:822:LYS:HA	1:A:825:PHE:HD2	1.71	0.56
1:B:49:LEU:HD11	1:B:64:LEU:HD12	1.88	0.56
1:B:379:LYS:O	1:B:383:SER:OG	2.23	0.56
1:A:833:ARG:HG3	1:A:838:LEU:HG	1.87	0.56
1:A:1205:VAL:HG11	1:A:1283:LYS:HE2	1.88	0.56
1:A:1272:GLN:HB2	1:A:1278:GLU:HG3	1.88	0.56
1:B:676:TYR:OH	1:B:704:THR:OG1	2.18	0.56
1:A:1011:ASP:OD2	1:A:1030:VAL:HG13	2.06	0.55
1:B:1011:ASP:OD2	1:B:1030:VAL:HG13	2.06	0.55
1:B:1223:MET:HG3	1:B:1256:PHE:HB3	1.87	0.55
1:B:1272:GLN:HB2	1:B:1278:GLU:HG3	1.88	0.55
1:A:379:LYS:O	1:A:383:SER:OG	2.23	0.55
1:B:366:GLN:HB2	1:B:367:PRO:CD	2.37	0.55
1:B:822:LYS:HA	1:B:825:PHE:HD2	1.70	0.55
1:A:1080:TYR:CE2	1:A:1266:PRO:HG3	2.42	0.55
1:B:1041:ILE:HD11	1:B:1085:ALA:HB3	1.88	0.55
1:A:315:THR:HG23	1:A:924:GLN:HB3	1.88	0.55
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.88	0.55
1:A:1041:ILE:HD11	1:A:1085:ALA:HB3	1.89	0.55
1:B:315:THR:HG23	1:B:924:GLN:HB3	1.88	0.55
1:B:1003:LEU:HB2	1:B:1038:HIS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1283:LYS:O	1:B:1287:LEU:HG	2.07	0.55
1:A:470:VAL:O	1:A:501:PHE:HB2	2.07	0.55
1:A:366:GLN:HB2	1:A:367:PRO:CD	2.37	0.55
1:B:1362:TYR:CD1	1:B:1362:TYR:C	2.81	0.55
1:A:1296:ASP:HA	1:A:1366:LEU:HB2	1.89	0.54
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.81	0.54
1:B:1235:ILE:O	1:B:1239:LEU:HG	2.08	0.54
1:A:1362:TYR:C	1:A:1362:TYR:HD1	2.10	0.54
1:B:807:ASN:O	1:B:864:SER:OG	2.26	0.54
1:A:49:LEU:HD11	1:A:64:LEU:HD12	1.89	0.54
1:A:1108:VAL:HA	1:A:1136:PRO:HB3	1.87	0.54
1:B:1362:TYR:C	1:B:1362:TYR:HD1	2.10	0.54
1:B:380:LEU:HG	1:B:865:VAL:HG13	1.88	0.54
1:B:1080:TYR:CE2	1:B:1266:PRO:HG3	2.42	0.54
1:A:144:ILE:HG13	1:A:183:VAL:HB	1.89	0.53
1:A:325:LEU:HA	1:A:330:VAL:HG21	1.89	0.53
1:B:355:LEU:HB2	1:B:360:LEU:HD11	1.89	0.53
1:B:355:LEU:HD13	1:B:912:PHE:CZ	2.44	0.53
1:A:1235:ILE:O	1:A:1239:LEU:HG	2.08	0.53
1:A:1283:LYS:O	1:A:1287:LEU:HG	2.07	0.53
1:B:470:VAL:O	1:B:501:PHE:HB2	2.08	0.53
1:A:1107:SER:HB3	1:A:1120:ASP:HA	1.91	0.53
1:A:355:LEU:HB2	1:A:360:LEU:HD11	1.89	0.53
1:A:89:LEU:HA	1:A:94:HIS:CD2	2.43	0.53
1:A:807:ASN:O	1:A:864:SER:OG	2.26	0.53
1:B:89:LEU:HA	1:B:94:HIS:CD2	2.43	0.53
1:B:144:ILE:HG13	1:B:183:VAL:HB	1.91	0.53
1:B:869:SER:HB2	1:B:886:ARG:HD2	1.90	0.53
1:A:1003:LEU:HB2	1:A:1038:HIS:HB2	1.90	0.53
1:A:610:GLU:O	1:A:1050:GLY:HA2	2.09	0.52
1:A:741:ASP:HB2	1:A:744:ARG:HB2	1.89	0.52
1:B:998:VAL:O	1:B:999:PRO:O	2.27	0.52
1:B:113:THR:N	1:B:114:PRO:HD2	2.25	0.52
1:A:869:SER:HB2	1:A:886:ARG:HD2	1.90	0.52
1:B:292:ALA:HA	1:B:295:MET:SD	2.50	0.52
1:A:113:THR:N	1:A:114:PRO:HD2	2.25	0.52
1:A:747:SER:HB3	1:A:784:TYR:HB3	1.92	0.52
1:B:960:TYR:O	1:B:961:ARG:HG2	2.10	0.52
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.43	0.52
1:B:325:LEU:HA	1:B:330:VAL:HG21	1.90	0.52
1:A:177:CYS:HB3	1:A:205:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:SER:HB2	1:A:1306:ILE:HG23	1.92	0.52
1:B:345:PHE:HB3	1:B:893:TRP:CE2	2.45	0.52
1:B:741:ASP:HB2	1:B:744:ARG:HB2	1.90	0.52
1:A:960:TYR:O	1:A:961:ARG:HG2	2.10	0.52
1:A:998:VAL:O	1:A:999:PRO:O	2.27	0.52
1:B:610:GLU:O	1:B:1050:GLY:HA2	2.10	0.52
1:B:1107:SER:HB3	1:B:1120:ASP:HA	1.91	0.52
1:B:572:PHE:HA	1:B:577:HIS:ND1	2.25	0.51
1:B:1108:VAL:HB	1:B:1122:THR:HA	1.92	0.51
1:A:998:VAL:CG2	1:A:999:PRO:HD2	2.41	0.51
1:B:1221:SER:HB2	1:B:1306:ILE:HG23	1.92	0.51
1:A:292:ALA:HA	1:A:295:MET:SD	2.51	0.51
1:A:572:PHE:HA	1:A:577:HIS:ND1	2.26	0.51
1:B:858:SER:HA	1:B:861:LYS:HD2	1.92	0.51
1:B:1216:ASN:HA	1:B:1219:MET:SD	2.51	0.51
1:A:1108:VAL:HB	1:A:1122:THR:HA	1.93	0.51
1:A:1228:HIS:NE2	1:A:1310:ASP:OD1	2.44	0.51
1:A:858:SER:HA	1:A:861:LYS:HD2	1.92	0.50
1:B:747:SER:HB3	1:B:784:TYR:HB3	1.93	0.50
1:B:177:CYS:HB3	1:B:205:ALA:HB1	1.92	0.50
1:B:998:VAL:CG2	1:B:999:PRO:HD2	2.41	0.50
1:B:1200:ILE:CD1	1:B:1228:HIS:CD2	2.95	0.50
1:B:1226:THR:OG1	1:B:1228:HIS:CD2	2.65	0.50
1:B:1228:HIS:NE2	1:B:1310:ASP:OD1	2.44	0.50
1:A:1226:THR:OG1	1:A:1228:HIS:CD2	2.65	0.50
1:A:345:PHE:HB3	1:A:893:TRP:CE2	2.45	0.50
1:A:1216:ASN:HA	1:A:1219:MET:SD	2.51	0.50
1:B:208:GLY:HA3	1:B:782:VAL:HB	1.94	0.49
1:A:352:VAL:HG13	1:A:359:HIS:CD2	2.47	0.49
1:B:352:VAL:HG13	1:B:359:HIS:CD2	2.46	0.49
1:B:989:GLU:HA	1:B:1017:ARG:HG2	1.95	0.49
1:A:208:GLY:HA3	1:A:782:VAL:HB	1.94	0.49
1:A:387:LEU:HD21	1:A:861:LYS:HD3	1.95	0.49
1:A:560:ARG:N	1:A:561:PRO:HD3	2.28	0.49
1:B:108:SER:OG	1:B:965:SER:O	2.21	0.49
1:B:1080:TYR:OH	1:B:1082:GLN:NE2	2.42	0.49
1:B:1282:TYR:O	1:B:1286:PHE:O	2.31	0.49
1:B:1108:VAL:HG13	1:B:1136:PRO:HG3	1.95	0.49
1:A:1200:ILE:CD1	1:A:1228:HIS:CD2	2.95	0.49
1:B:1099:SER:O	1:B:1103:PHE:O	2.30	0.49
1:B:1307:VAL:HG11	1:B:1311:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLY:O	1:A:605:PHE:O	2.32	0.48
1:A:811:LEU:HD11	1:A:828:PHE:CE2	2.48	0.48
1:B:560:ARG:N	1:B:561:PRO:HD3	2.29	0.48
1:B:697:ARG:HA	1:B:700:TRP:CE3	2.48	0.48
1:B:811:LEU:HD11	1:B:828:PHE:CE2	2.48	0.48
1:A:1099:SER:O	1:A:1103:PHE:O	2.30	0.48
1:A:1282:TYR:O	1:A:1286:PHE:O	2.31	0.48
1:B:92:ASP:OD1	1:B:92:ASP:N	2.46	0.48
1:B:387:LEU:HD21	1:B:861:LYS:HD3	1.96	0.48
1:B:105:LEU:HD11	1:B:932:VAL:HG12	1.96	0.48
1:A:1047:GLU:HA	1:A:1138:LEU:O	2.14	0.48
1:B:1239:LEU:HB2	1:B:1244:LYS:HE3	1.96	0.48
1:A:53:ALA:HB1	1:A:60:TYR:HA	1.95	0.48
1:A:366:GLN:O	1:A:370:LEU:HB2	2.14	0.48
1:B:53:ALA:HB1	1:B:60:TYR:HA	1.96	0.48
1:B:1030:VAL:HG12	1:B:1032:ALA:H	1.79	0.48
1:A:92:ASP:N	1:A:92:ASP:OD1	2.46	0.48
1:A:1030:VAL:HG12	1:A:1032:ALA:H	1.79	0.48
1:A:1239:LEU:HB2	1:A:1244:LYS:HE3	1.96	0.48
1:B:366:GLN:O	1:B:370:LEU:HB2	2.14	0.48
1:B:1047:GLU:HA	1:B:1138:LEU:O	2.14	0.48
1:A:989:GLU:HA	1:A:1017:ARG:HG2	1.95	0.48
1:B:724:PHE:HA	1:B:822:LYS:HE2	1.95	0.48
1:B:1040:LEU:O	1:B:1131:GLY:HA2	2.14	0.48
1:A:1073:ILE:HG12	1:A:1289:VAL:HG12	1.96	0.47
1:A:724:PHE:HA	1:A:822:LYS:HE2	1.95	0.47
1:B:604:GLY:O	1:B:605:PHE:O	2.31	0.47
1:B:97:PRO:O	1:B:937:GLU:OE1	2.33	0.47
1:B:1280:TRP:HB3	1:B:1395:LEU:HG	1.95	0.47
1:A:724:PHE:HA	1:A:822:LYS:CE	2.44	0.47
1:B:724:PHE:HA	1:B:822:LYS:CE	2.44	0.47
1:B:791:PHE:CZ	1:B:797:MET:SD	3.07	0.47
1:B:1073:ILE:HG12	1:B:1289:VAL:HG12	1.97	0.47
1:A:1108:VAL:HG13	1:A:1136:PRO:HG3	1.96	0.47
1:A:1307:VAL:HG11	1:A:1311:MET:SD	2.54	0.47
1:A:1376:ASP:N	1:A:1376:ASP:OD1	2.47	0.47
1:B:703:LEU:HD12	1:B:806:LEU:HB2	1.97	0.47
1:B:1376:ASP:OD1	1:B:1376:ASP:N	2.47	0.47
1:A:176:PHE:CD2	1:A:205:ALA:HB3	2.50	0.47
1:A:697:ARG:HA	1:A:700:TRP:CE3	2.49	0.47
1:B:176:PHE:CD2	1:B:205:ALA:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LEU:N	1:B:644:PRO:HD2	2.30	0.47
1:A:97:PRO:O	1:A:937:GLU:OE1	2.33	0.46
1:A:791:PHE:CZ	1:A:797:MET:SD	3.08	0.46
1:A:1280:TRP:HB3	1:A:1395:LEU:HG	1.95	0.46
1:A:986:VAL:HG22	1:A:987:PRO:HD2	1.97	0.46
1:A:1040:LEU:O	1:A:1131:GLY:HA2	2.14	0.46
1:A:167:LEU:HA	1:A:184:ILE:HD11	1.96	0.46
1:A:643:LEU:N	1:A:644:PRO:HD2	2.30	0.46
1:A:1001:ALA:HB1	1:A:1040:LEU:HB2	1.97	0.46
1:B:186:TYR:HE1	1:B:215:ARG:HD2	1.81	0.46
1:B:723:ARG:HA	1:B:726:LYS:HE3	1.97	0.46
1:B:1001:ALA:HB1	1:B:1040:LEU:HB2	1.97	0.46
1:A:105:LEU:HD11	1:A:932:VAL:HG12	1.96	0.46
1:A:713:GLU:HB3	1:A:816:SER:HA	1.98	0.46
1:A:767:LEU:HA	1:A:770:GLU:HG2	1.97	0.46
1:A:1134:LEU:C	1:A:1136:PRO:HD3	2.36	0.46
1:B:713:GLU:HB3	1:B:816:SER:HA	1.98	0.46
1:B:104:LYS:HB3	1:B:968:PRO:HD3	1.98	0.46
1:B:167:LEU:HA	1:B:184:ILE:HD11	1.96	0.46
1:B:1134:LEU:C	1:B:1136:PRO:HD3	2.36	0.46
1:B:1201:ASN:O	1:B:1202:ILE:HG13	2.16	0.46
1:A:1200:ILE:HD11	1:A:1312:TYR:HD1	1.81	0.45
1:A:723:ARG:HA	1:A:726:LYS:HE3	1.97	0.45
1:B:560:ARG:N	1:B:561:PRO:CD	2.80	0.45
1:A:969:SER:HB2	1:A:977:LYS:HD3	1.98	0.45
1:A:1046:ARG:HE	1:A:1137:ARG:HG2	1.80	0.45
1:B:961:ARG:HG2	1:B:983:PHE:CE2	2.52	0.45
1:B:1046:ARG:HE	1:B:1137:ARG:HG2	1.80	0.45
1:A:186:TYR:HE1	1:A:215:ARG:HD2	1.81	0.45
1:A:702:ALA:HA	1:A:732:ARG:HB3	1.99	0.45
1:A:1080:TYR:OH	1:A:1082:GLN:NE2	2.42	0.45
1:A:45:LEU:HD12	1:A:81:LEU:HD21	1.99	0.45
1:A:119:HIS:NE2	1:A:172:PHE:CD1	2.85	0.45
1:A:573:ILE:HG22	1:A:574:SER:H	1.81	0.45
1:A:998:VAL:HG21	1:A:1002:TRP:CE3	2.52	0.45
1:A:1201:ASN:O	1:A:1202:ILE:HG13	2.16	0.45
1:B:767:LEU:HA	1:B:770:GLU:HG2	1.98	0.45
1:A:108:SER:OG	1:A:965:SER:O	2.21	0.45
1:A:900:PHE:CZ	1:A:943:VAL:HB	2.52	0.45
1:A:1241:PRO:O	1:A:1245:ASP:OD1	2.35	0.45
1:B:66:ARG:HB2	1:B:72:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:VAL:HG22	1:B:987:PRO:HD2	1.99	0.45
1:B:998:VAL:HG21	1:B:1002:TRP:CE3	2.52	0.45
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.52	0.45
1:B:900:PHE:CZ	1:B:943:VAL:HB	2.52	0.45
1:B:1008:VAL:HB	1:B:1033:ILE:HB	1.99	0.45
1:A:66:ARG:HB2	1:A:72:PHE:CE2	2.52	0.45
1:A:560:ARG:N	1:A:561:PRO:CD	2.80	0.45
1:B:45:LEU:HD12	1:B:81:LEU:HD21	1.99	0.45
1:B:119:HIS:NE2	1:B:172:PHE:CD1	2.85	0.45
1:B:382:LYS:HG2	1:B:385:LEU:HD21	1.98	0.45
1:A:104:LYS:HB3	1:A:968:PRO:HD3	1.99	0.45
1:A:616:VAL:HA	1:A:619:HIS:CD2	2.52	0.45
1:B:573:ILE:HG22	1:B:574:SER:H	1.81	0.44
1:B:969:SER:HB2	1:B:977:LYS:HD3	1.98	0.44
1:B:1241:PRO:O	1:B:1245:ASP:OD1	2.35	0.44
1:A:382:LYS:HG2	1:A:385:LEU:HD21	1.98	0.44
1:B:702:ALA:HA	1:B:732:ARG:HB3	2.00	0.44
1:A:703:LEU:HD12	1:A:806:LEU:HB2	1.98	0.44
1:A:732:ARG:HB2	1:A:856:PRO:HG2	1.99	0.44
1:B:128:GLU:N	1:B:129:PRO:HD2	2.33	0.44
1:B:732:ARG:HB2	1:B:856:PRO:HG2	1.99	0.44
1:A:1008:VAL:HB	1:A:1033:ILE:HB	2.00	0.44
1:B:89:LEU:HA	1:B:94:HIS:HB2	1.99	0.44
1:A:110:ARG:CZ	1:A:976:VAL:HG11	2.48	0.44
1:A:1265:TRP:HE1	1:A:1269:LEU:HG	1.83	0.44
1:B:589:GLU:OE1	1:B:589:GLU:HA	2.17	0.44
1:B:1378:LEU:HA	1:B:1381:GLN:HB2	2.00	0.44
1:A:89:LEU:HA	1:A:94:HIS:HB2	1.99	0.44
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.53	0.44
1:B:110:ARG:CZ	1:B:976:VAL:HG11	2.48	0.44
1:B:1200:ILE:HD11	1:B:1312:TYR:HD1	1.82	0.44
1:A:128:GLU:N	1:A:129:PRO:HD2	2.33	0.44
1:A:1081:PHE:HZ	1:A:1134:LEU:HB2	1.82	0.44
1:A:1297:LYS:HD2	1:A:1315:VAL:HG13	1.99	0.43
1:A:1399:LEU:N	1:A:1400:PRO:HD2	2.32	0.43
1:B:616:VAL:HA	1:B:619:HIS:CD2	2.52	0.43
1:B:1081:PHE:HZ	1:B:1134:LEU:HB2	1.82	0.43
1:B:1399:LEU:N	1:B:1400:PRO:HD2	2.32	0.43
1:A:380:LEU:HD13	1:A:868:LEU:HD22	2.00	0.43
1:B:90:ARG:HG3	1:B:100:LEU:HD11	2.00	0.43
1:B:144:ILE:HD13	1:B:154:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:ASP:OD1	1:B:1148:ASP:O	2.36	0.43
1:B:1205:VAL:HG21	1:B:1279:ILE:HG23	2.00	0.43
1:B:1297:LYS:HD2	1:B:1315:VAL:HG13	1.99	0.43
1:A:144:ILE:HD13	1:A:154:LEU:HD21	2.00	0.43
1:B:380:LEU:HD13	1:B:868:LEU:HD22	2.01	0.43
1:B:572:PHE:N	1:B:572:PHE:CD1	2.86	0.43
1:A:208:GLY:HA3	1:A:782:VAL:CG1	2.49	0.43
1:A:572:PHE:N	1:A:572:PHE:CD1	2.87	0.43
1:B:532:TYR:O	1:B:536:SER:N	2.47	0.43
1:B:37:ALA:HB3	1:B:227:LEU:HB3	2.01	0.43
1:A:67:ILE:HB	1:A:194:PHE:HZ	1.84	0.43
1:B:53:ALA:HB2	1:B:59:ILE:HG22	2.00	0.43
1:B:97:PRO:HA	1:B:100:LEU:HG	1.99	0.43
1:A:1105:LEU:O	1:A:1105:LEU:HD12	2.19	0.43
1:B:154:LEU:O	1:B:155:ASP:CG	2.57	0.43
1:B:654:ARG:NH1	1:B:824:ASP:OD2	2.52	0.43
1:A:505:THR:N	1:A:506:PRO:HD3	2.34	0.43
1:B:554:ILE:HG21	1:B:568:PHE:CE1	2.54	0.43
1:A:154:LEU:O	1:A:155:ASP:CG	2.56	0.43
1:A:1148:ASP:OD1	1:A:1148:ASP:O	2.36	0.43
1:A:37:ALA:HB3	1:A:227:LEU:HB3	2.00	0.42
1:B:505:THR:N	1:B:506:PRO:HD3	2.34	0.42
1:B:1265:TRP:HE1	1:B:1269:LEU:HG	1.83	0.42
1:A:654:ARG:NH1	1:A:824:ASP:OD2	2.52	0.42
1:A:1378:LEU:HA	1:A:1381:GLN:HB2	2.00	0.42
1:B:673:ASN:OD1	1:B:677:ILE:HD12	2.20	0.42
1:B:1119:ASP:C	1:B:1121:ASN:H	2.23	0.42
1:A:53:ALA:HB2	1:A:59:ILE:HG22	2.01	0.42
1:A:97:PRO:HA	1:A:100:LEU:HG	2.00	0.42
1:A:998:VAL:O	1:A:999:PRO:C	2.58	0.42
1:A:1060:VAL:HB	1:A:1093:ARG:HG2	2.00	0.42
1:B:67:ILE:HB	1:B:194:PHE:HZ	1.84	0.42
1:B:208:GLY:HA3	1:B:782:VAL:CG1	2.49	0.42
1:B:936:LEU:HB2	1:B:939:VAL:HG21	2.02	0.42
1:B:998:VAL:O	1:B:999:PRO:C	2.58	0.42
1:A:90:ARG:HG3	1:A:100:LEU:HD11	2.01	0.42
1:B:682:LEU:HD13	1:B:788:LEU:HB2	2.01	0.42
1:A:1116:ILE:HG22	1:A:1118:GLY:H	1.85	0.42
1:A:1403:MET:HB3	1:A:1406:THR:OG1	2.20	0.42
1:A:682:LEU:HD22	1:A:788:LEU:HA	2.02	0.42
1:A:1203:PHE:CD2	1:A:1300:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:HG	1:B:849:LEU:HD22	2.01	0.42
1:B:747:SER:HB2	1:B:781:ASP:HB3	2.02	0.42
1:B:1103:PHE:CD1	1:B:1138:LEU:HD22	2.55	0.42
1:B:1206:ALA:HB3	1:B:1239:LEU:CD2	2.50	0.42
1:A:747:SER:HB2	1:A:781:ASP:HB3	2.01	0.42
1:A:1119:ASP:C	1:A:1121:ASN:H	2.23	0.42
1:B:143:LEU:HD23	1:B:184:ILE:HD12	2.02	0.42
1:B:332:ALA:HB1	1:B:334:PHE:CE2	2.55	0.42
1:B:1060:VAL:HB	1:B:1093:ARG:HG2	2.00	0.42
1:A:204:LEU:HG	1:A:210:ALA:HB3	2.02	0.42
1:A:689:ILE:HD11	1:A:760:LEU:HD13	2.02	0.42
1:B:335:GLU:HB3	1:B:897:TYR:HB3	2.02	0.42
1:B:1116:ILE:HG22	1:B:1118:GLY:H	1.84	0.42
1:A:109:LEU:HA	1:A:230:ASN:HD21	1.85	0.41
1:B:371:VAL:HA	1:B:374:LEU:HG	2.02	0.41
1:A:490:PHE:HB3	1:A:499:PHE:CE2	2.56	0.41
1:A:1205:VAL:HG21	1:A:1279:ILE:HG23	2.02	0.41
1:B:109:LEU:HA	1:B:230:ASN:HD21	1.85	0.41
1:A:403:VAL:C	1:A:405:HIS:H	2.24	0.41
1:B:427:VAL:HG21	1:B:587:TRP:HB3	2.01	0.41
1:B:572:PHE:N	1:B:572:PHE:HD1	2.18	0.41
1:B:1105:LEU:HD12	1:B:1105:LEU:O	2.20	0.41
1:A:589:GLU:HA	1:A:589:GLU:OE1	2.19	0.41
1:B:204:LEU:HG	1:B:210:ALA:HB3	2.02	0.41
1:B:400:HIS:HE2	1:B:847:LEU:HD13	1.86	0.41
1:B:403:VAL:C	1:B:405:HIS:H	2.24	0.41
1:B:423:GLU:O	1:B:424:GLU:HB2	2.20	0.41
1:B:1403:MET:HB3	1:B:1406:THR:OG1	2.20	0.41
1:A:1204:SER:HB3	1:A:1215:LEU:HD12	2.03	0.41
1:B:951:ILE:HG21	1:B:955:PRO:HG3	2.01	0.41
1:B:1203:PHE:CD2	1:B:1300:PHE:HB2	2.55	0.41
1:B:1250:MET:HG3	1:B:1256:PHE:CZ	2.56	0.41
1:A:423:GLU:O	1:A:424:GLU:HB2	2.21	0.41
1:A:1103:PHE:CD1	1:A:1138:LEU:HD22	2.55	0.41
1:A:1107:SER:CB	1:A:1120:ASP:HA	2.50	0.41
1:A:1206:ALA:HB3	1:A:1239:LEU:CD2	2.50	0.41
1:A:1378:LEU:HD22	1:A:1399:LEU:HD23	2.02	0.41
1:B:39:PHE:CE2	1:B:227:LEU:HD22	2.56	0.41
1:B:682:LEU:HD22	1:B:788:LEU:HA	2.01	0.41
1:A:39:PHE:CE2	1:A:227:LEU:HD22	2.55	0.41
1:A:342:ARG:HG2	1:A:347:PRO:CA	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LEU:O	1:A:492:LYS:HB2	2.21	0.41
1:A:1201:ASN:HB3	1:A:1233:TRP:NE1	2.33	0.41
1:B:176:PHE:HB3	1:B:212:TYR:HB3	2.02	0.41
1:B:231:GLY:HA2	1:B:964:LEU:CD1	2.50	0.41
1:B:490:PHE:HB3	1:B:499:PHE:CE2	2.55	0.41
1:A:231:GLY:HA2	1:A:964:LEU:CD1	2.51	0.41
1:A:335:GLU:HB3	1:A:897:TYR:HB3	2.02	0.41
1:A:682:LEU:HD13	1:A:788:LEU:HB2	2.01	0.41
1:B:1200:ILE:O	1:B:1230:VAL:HA	2.21	0.41
1:B:1399:LEU:N	1:B:1400:PRO:CD	2.84	0.41
1:A:427:VAL:HG21	1:A:587:TRP:HB3	2.02	0.41
1:A:554:ILE:O	1:A:558:SER:HB2	2.21	0.41
1:A:673:ASN:OD1	1:A:677:ILE:HD12	2.20	0.41
1:A:893:TRP:HB3	1:A:944:PHE:CZ	2.56	0.41
1:B:195:ALA:HB3	1:B:196:PRO:HD3	2.03	0.41
1:B:998:VAL:HG22	1:B:999:PRO:HD2	2.02	0.41
1:B:1132:THR:O	1:B:1134:LEU:HG	2.21	0.41
1:A:936:LEU:HB2	1:A:939:VAL:HG21	2.02	0.41
1:B:465:VAL:HG22	1:B:643:LEU:HD13	2.03	0.41
1:B:488:LEU:O	1:B:492:LYS:HB2	2.21	0.41
1:A:143:LEU:HD23	1:A:184:ILE:HD12	2.02	0.40
1:A:572:PHE:N	1:A:572:PHE:HD1	2.18	0.40
1:B:427:VAL:HG13	1:B:428:ILE:H	1.86	0.40
1:A:961:ARG:HG2	1:A:983:PHE:CZ	2.56	0.40
1:B:1246:PHE:HA	1:B:1249:HIS:ND1	2.36	0.40
1:A:332:ALA:HB1	1:A:334:PHE:CE2	2.56	0.40
1:A:420:ASP:HA	1:A:423:GLU:OE1	2.21	0.40
1:A:1246:PHE:HA	1:A:1249:HIS:ND1	2.36	0.40
1:B:420:ASP:HA	1:B:423:GLU:OE1	2.21	0.40
1:B:689:ILE:HD11	1:B:760:LEU:HD13	2.02	0.40
1:B:961:ARG:HG2	1:B:983:PHE:CZ	2.56	0.40
1:B:1201:ASN:CB	1:B:1233:TRP:HE1	2.30	0.40
1:B:1378:LEU:HD22	1:B:1399:LEU:HD23	2.02	0.40
1:A:389:LEU:HG	1:A:849:LEU:HD22	2.02	0.40
1:A:600:VAL:HG12	1:A:601:PHE:N	2.36	0.40
1:A:1053:ALA:HA	1:A:1054:PRO:HD3	1.92	0.40
1:A:1132:THR:O	1:A:1134:LEU:HG	2.21	0.40
1:A:1250:MET:HG3	1:A:1256:PHE:CZ	2.56	0.40
1:B:382:LYS:HA	1:B:385:LEU:CG	2.37	0.40
1:A:53:ALA:HB2	1:A:63:LEU:HD12	2.03	0.40
1:A:400:HIS:HE2	1:A:847:LEU:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:VAL:HB	1:A:461:ILE:HD12	2.04	0.40
1:B:554:ILE:O	1:B:558:SER:HB2	2.22	0.40
1:B:1201:ASN:HB3	1:B:1233:TRP:NE1	2.33	0.40
1:B:1231:LYS:HE3	1:B:1257:LYS:HD2	2.03	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	1246/1382 (90%)	988 (79%)	208 (17%)	50 (4%)	3	26
1	B	1246/1382 (90%)	989 (79%)	207 (17%)	50 (4%)	3	26
All	All	2492/2764 (90%)	1977 (79%)	415 (17%)	100 (4%)	3	26

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	A	424	GLU
1	A	427	VAL
1	A	506	PRO
1	A	541	SER
1	A	592	ARG
1	A	605	PHE
1	A	651	ALA
1	A	880	ASP
1	A	972	GLU
1	A	999	PRO
1	A	1067	PRO
1	A	1236	GLU
1	B	155	ASP

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Mol	Chain	Res	Type
1	B	424	GLU
1	B	427	VAL
1	B	506	PRO
1	B	541	SER
1	B	592	ARG
1	B	605	PHE
1	B	651	ALA
1	B	880	ASP
1	B	999	PRO
1	B	1067	PRO
1	B	1236	GLU
1	A	163	GLY
1	A	329	ASN
1	A	331	SER
1	A	367	PRO
1	A	508	GLY
1	A	572	PHE
1	A	578	GLU
1	A	881	ASN
1	A	1146	GLU
1	B	163	GLY
1	B	329	ASN
1	B	331	SER
1	B	367	PRO
1	B	508	GLY
1	B	572	PHE
1	B	578	GLU
1	B	881	ASN
1	B	972	GLU
1	B	1146	GLU
1	A	99	ALA
1	A	131	LEU
1	A	347	PRO
1	A	569	LYS
1	A	611	ASP
1	A	666	GLU
1	A	714	GLY
1	A	776	GLY
1	A	857	LEU
1	A	893	TRP
1	B	99	ALA
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	347	PRO
1	B	569	LYS
1	B	611	ASP
1	B	666	GLU
1	B	714	GLY
1	B	776	GLY
1	B	857	LEU
1	B	893	TRP
1	A	154	LEU
1	A	566	LEU
1	A	671	ASN
1	A	677	ILE
1	A	692	SER
1	A	1049	PRO
1	A	1097	GLY
1	A	1109	GLY
1	A	1270	ARG
1	B	154	LEU
1	B	566	LEU
1	B	671	ASN
1	B	677	ILE
1	B	692	SER
1	B	1049	PRO
1	B	1097	GLY
1	B	1109	GLY
1	B	1270	ARG
1	A	1127	MET
1	B	568	PHE
1	B	1311	MET
1	A	137	GLY
1	A	568	PHE
1	A	1098	ARG
1	A	1311	MET
1	B	137	GLY
1	B	1098	ARG
1	B	1127	MET
1	A	93	GLY
1	A	388	GLY
1	A	409	GLY
1	B	388	GLY
1	B	409	GLY
1	A	326	GLY

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Mol	Chain	Res	Type
1	B	93	GLY
1	B	326	GLY

### 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	1097/1197 (92%)	961 (88%)	136 (12%)	4	21
1	B	1097/1197 (92%)	960 (88%)	137 (12%)	4	21
All	All	2194/2394 (92%)	1921 (88%)	273 (12%)	4	21

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	49	LEU
1	A	56	ASN
1	A	64	LEU
1	A	67	ILE
1	A	81	LEU
1	A	82	TYR
1	A	90	ARG
1	A	92	ASP
1	A	109	LEU
1	A	123	TYR
1	A	158	HIS
1	A	175	LYS
1	A	178	VAL
1	A	181	ARG
1	A	183	VAL
1	A	192	LYS
1	A	194	PHE
1	A	203	ASP
1	A	204	LEU
1	A	213	ARG

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Mol	Chain	Res	Type
1	A	222	HIS
1	A	243	TYR
1	A	300	PHE
1	A	315	THR
1	A	342	ARG
1	A	372	ASP
1	A	378	ARG
1	A	396	ASP
1	A	442	SER
1	A	453	HIS
1	A	460	GLN
1	A	462	ARG
1	A	479	ASP
1	A	521	LEU
1	A	522	GLU
1	A	534	GLU
1	A	539	GLU
1	A	550	PHE
1	A	554	ILE
1	A	555	LYS
1	A	572	PHE
1	A	573	ILE
1	A	576	LYS
1	A	585	LYS
1	A	605	PHE
1	A	609	ARG
1	A	612	ASN
1	A	617	MET
1	A	620	ARG
1	A	624	ASP
1	A	633	TYR
1	A	641	MET
1	A	662	GLU
1	A	663	ASP
1	A	667	LEU
1	A	668	THR
1	A	670	LEU
1	A	672	VAL
1	A	676	TYR
1	A	680	HIS
1	A	686	VAL
1	A	709	LEU

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Mol	Chain	Res	Type
1	A	729	ASP
1	A	734	ASP
1	A	741	ASP
1	A	753	LEU
1	A	758	ASP
1	A	761	LEU
1	A	767	LEU
1	A	769	LEU
1	A	779	GLU
1	A	785	ASP
1	A	791	PHE
1	A	801	ASP
1	A	809	ARG
1	A	840	VAL
1	A	868	LEU
1	A	886	ARG
1	A	889	LEU
1	A	893	TRP
1	A	941	LEU
1	A	944	PHE
1	A	945	LEU
1	A	948	THR
1	A	951	ILE
1	A	953	GLU
1	A	958	ARG
1	A	960	TYR
1	A	962	TYR
1	A	979	LEU
1	A	986	VAL
1	A	997	ASP
1	A	1010	VAL
1	A	1012	ASP
1	A	1016	LEU
1	A	1034	TYR
1	A	1037	GLU
1	A	1045	SER
1	A	1046	ARG
1	A	1068	HIS
1	A	1071	ASP
1	A	1094	LEU
1	A	1103	PHE
1	A	1105	LEU

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Mol	Chain	Res	Type
1	A	1106	GLU
1	A	1120	ASP
1	A	1122	THR
1	A	1128	ASP
1	A	1132	THR
1	A	1147	GLU
1	A	1150	LEU
1	A	1203	PHE
1	A	1204	SER
1	A	1211	TYR
1	A	1214	MET
1	A	1215	LEU
1	A	1218	MET
1	A	1224	HIS
1	A	1228	HIS
1	A	1234	PHE
1	A	1245	ASP
1	A	1246	PHE
1	A	1254	TYR
1	A	1258	TYR
1	A	1265	TRP
1	A	1290	LEU
1	A	1291	PHE
1	A	1312	TYR
1	A	1362	TYR
1	A	1364	VAL
1	A	1369	PHE
1	A	1376	ASP
1	A	1381	GLN
1	A	1395	LEU
1	A	1401	ASN
1	B	48	LEU
1	B	49	LEU
1	B	56	ASN
1	B	64	LEU
1	B	67	ILE
1	B	81	LEU
1	B	82	TYR
1	B	90	ARG
1	B	92	ASP
1	B	109	LEU
1	B	123	TYR

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Mol	Chain	Res	Type
1	B	158	HIS
1	B	175	LYS
1	B	178	VAL
1	B	181	ARG
1	B	183	VAL
1	B	192	LYS
1	B	194	PHE
1	B	203	ASP
1	B	204	LEU
1	B	213	ARG
1	B	222	HIS
1	B	243	TYR
1	B	300	PHE
1	B	315	THR
1	B	342	ARG
1	B	372	ASP
1	B	378	ARG
1	B	442	SER
1	B	453	HIS
1	B	460	GLN
1	B	462	ARG
1	B	479	ASP
1	B	521	LEU
1	B	522	GLU
1	B	534	GLU
1	B	539	GLU
1	B	550	PHE
1	B	554	ILE
1	B	555	LYS
1	B	572	PHE
1	B	573	ILE
1	B	576	LYS
1	B	585	LYS
1	B	589	GLU
1	B	605	PHE
1	B	609	ARG
1	B	612	ASN
1	B	617	MET
1	B	620	ARG
1	B	624	ASP
1	B	633	TYR
1	B	641	MET

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Mol	Chain	Res	Type
1	B	656	ASN
1	B	662	GLU
1	B	663	ASP
1	B	667	LEU
1	B	668	THR
1	B	670	LEU
1	B	672	VAL
1	B	676	TYR
1	B	680	HIS
1	B	686	VAL
1	B	709	LEU
1	B	729	ASP
1	B	734	ASP
1	B	741	ASP
1	B	753	LEU
1	B	758	ASP
1	B	761	LEU
1	B	767	LEU
1	B	769	LEU
1	B	779	GLU
1	B	785	ASP
1	B	791	PHE
1	B	801	ASP
1	B	809	ARG
1	B	840	VAL
1	B	868	LEU
1	B	881	ASN
1	B	886	ARG
1	B	889	LEU
1	B	893	TRP
1	B	941	LEU
1	B	944	PHE
1	B	945	LEU
1	B	948	THR
1	B	951	ILE
1	B	953	GLU
1	B	958	ARG
1	B	960	TYR
1	B	962	TYR
1	B	979	LEU
1	B	986	VAL
1	B	997	ASP

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Mol	Chain	Res	Type
1	B	1012	ASP
1	B	1016	LEU
1	B	1034	TYR
1	B	1037	GLU
1	B	1045	SER
1	B	1046	ARG
1	B	1068	HIS
1	B	1071	ASP
1	B	1094	LEU
1	B	1103	PHE
1	B	1105	LEU
1	B	1106	GLU
1	B	1120	ASP
1	B	1122	THR
1	B	1128	ASP
1	B	1132	THR
1	B	1147	GLU
1	B	1150	LEU
1	B	1203	PHE
1	B	1204	SER
1	B	1211	TYR
1	B	1214	MET
1	B	1215	LEU
1	B	1218	MET
1	B	1224	HIS
1	B	1228	HIS
1	B	1234	PHE
1	B	1245	ASP
1	B	1246	PHE
1	B	1254	TYR
1	B	1258	TYR
1	B	1265	TRP
1	B	1290	LEU
1	B	1291	PHE
1	B	1312	TYR
1	B	1362	TYR
1	B	1364	VAL
1	B	1369	PHE
1	B	1376	ASP
1	B	1381	GLN
1	B	1395	LEU
1	B	1401	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	166	GLN
1	A	198	HIS
1	A	351	ASN
1	A	359	HIS
1	A	366	GLN
1	A	612	ASN
1	A	638	ASN
1	A	656	ASN
1	A	728	ASN
1	A	876	GLN
1	A	881	ASN
1	A	946	ASN
1	A	1038	HIS
1	A	1044	HIS
1	A	1082	GLN
1	A	1225	HIS
1	A	1227	ASN
1	A	1272	GLN
1	A	1397	GLN
1	B	94	HIS
1	B	166	GLN
1	B	198	HIS
1	B	351	ASN
1	B	359	HIS
1	B	366	GLN
1	B	612	ASN
1	B	638	ASN
1	B	656	ASN
1	B	728	ASN
1	B	876	GLN
1	B	881	ASN
1	B	946	ASN
1	B	1038	HIS
1	B	1044	HIS
1	B	1082	GLN
1	B	1225	HIS
1	B	1227	ASN
1	B	1272	GLN
1	B	1397	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1254/1382 (90%)	0.24	63 (5%) 28 25	73, 141, 251, 333	0
1	B	1254/1382 (90%)	0.50	121 (9%) 8 8	106, 188, 295, 398	0
All	All	2508/2764 (90%)	0.37	184 (7%) 15 13	73, 168, 272, 398	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	LYS	9.3
1	A	565	GLU	7.7
1	B	565	GLU	7.6
1	B	159	GLY	7.2
1	A	160	LYS	6.9
1	B	161	VAL	5.7
1	B	148	GLN	5.6
1	A	322	SER	5.2
1	A	325	LEU	5.0
1	B	1262	THR	5.0
1	B	1260	MET	4.7
1	B	162	LYS	4.4
1	B	1231	LYS	4.3
1	A	162	LYS	4.3
1	A	159	GLY	4.3
1	B	461	ILE	4.3
1	B	979	LEU	4.2
1	B	463	ARG	4.2
1	A	148	GLN	4.2
1	A	161	VAL	4.1
1	B	1399	LEU	4.1
1	A	324	SER	4.0
1	B	1392	LEU	4.0
1	B	1315	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	294	GLY	3.9
1	B	228	SER	3.9
1	B	576	LYS	3.9
1	B	1129	PHE	3.8
1	B	1128	ASP	3.8
1	B	1206	ALA	3.7
1	B	1400	PRO	3.7
1	A	446	SER	3.6
1	A	1260	MET	3.6
1	B	978	ALA	3.6
1	B	1055	ARG	3.6
1	B	713	GLU	3.6
1	A	1262	THR	3.6
1	A	1234	PHE	3.5
1	A	323	ASN	3.5
1	B	426	GLN	3.5
1	B	567	SER	3.4
1	B	166	GLN	3.4
1	B	1261	VAL	3.4
1	A	1231	LYS	3.4
1	B	1394	ASN	3.4
1	B	308	PHE	3.3
1	B	980	SER	3.3
1	B	879	PHE	3.2
1	A	1317	HIS	3.2
1	B	958	ARG	3.2
1	A	317	ASP	3.2
1	B	1197	HIS	3.1
1	B	1233	TRP	3.1
1	A	241	THR	3.1
1	B	165	ASP	3.1
1	B	389	LEU	3.1
1	B	434	LEU	3.1
1	A	142	PHE	3.0
1	B	96	ASP	3.0
1	B	446	SER	3.0
1	B	539	GLU	3.0
1	B	325	LEU	3.0
1	B	34	ALA	3.0
1	B	322	SER	3.0
1	B	1234	PHE	2.9
1	A	1385	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	432	ASN	2.9
1	B	875	PRO	2.9
1	B	410	ASP	2.9
1	A	1233	TRP	2.9
1	B	524	TYR	2.9
1	B	98	GLU	2.9
1	B	147	GLU	2.9
1	B	427	VAL	2.9
1	A	166	GLN	2.9
1	B	462	ARG	2.8
1	B	987	PRO	2.8
1	B	1232	PHE	2.8
1	A	872	SER	2.7
1	A	1201	ASN	2.7
1	B	1057	VAL	2.7
1	B	1127	MET	2.7
1	A	539	GLU	2.7
1	B	126	THR	2.7
1	B	566	LEU	2.7
1	A	42	PRO	2.7
1	B	1230	VAL	2.7
1	B	95	MET	2.7
1	B	1259	GLU	2.7
1	B	42	PRO	2.7
1	B	1058	GLN	2.7
1	A	1323	PRO	2.7
1	A	1261	VAL	2.7
1	A	320	LYS	2.6
1	A	713	GLU	2.6
1	A	566	LEU	2.6
1	B	628	LEU	2.6
1	A	293	LEU	2.6
1	A	319	PRO	2.6
1	B	1084	LYS	2.6
1	B	35	LEU	2.5
1	A	1206	ALA	2.5
1	B	1314	LEU	2.5
1	B	1037	GLU	2.5
1	B	1297	LYS	2.5
1	B	142	PHE	2.5
1	B	849	LEU	2.5
1	B	496	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1054	PRO	2.5
1	B	1205	VAL	2.4
1	B	363	ARG	2.4
1	B	915	VAL	2.4
1	A	447	ILE	2.4
1	A	1232	PHE	2.4
1	B	146	GLY	2.4
1	B	447	ILE	2.4
1	B	872	SER	2.4
1	A	1399	LEU	2.4
1	B	500	GLY	2.4
1	A	165	ASP	2.4
1	B	182	ASP	2.4
1	A	163	GLY	2.4
1	A	1395	LEU	2.4
1	B	1089	VAL	2.4
1	A	648	LEU	2.3
1	B	1130	GLN	2.3
1	A	1406	THR	2.3
1	B	957	LYS	2.3
1	A	1034	TYR	2.3
1	B	1407	ILE	2.3
1	A	523	ASN	2.3
1	B	235	GLU	2.3
1	A	564	VAL	2.3
1	B	444	SER	2.3
1	B	1098	ARG	2.3
1	A	576	LYS	2.3
1	B	1236	GLU	2.3
1	B	294	GLY	2.3
1	B	1254	TYR	2.3
1	A	141	TRP	2.3
1	A	1315	VAL	2.3
1	B	130	SER	2.2
1	A	389	LEU	2.2
1	B	1395	LEU	2.2
1	B	307	PRO	2.2
1	A	444	SER	2.2
1	B	969	SER	2.2
1	B	1237	GLN	2.2
1	B	955	PRO	2.2
1	A	1400	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1099	SER	2.2
1	B	1398	ASP	2.2
1	B	1391	SER	2.2
1	B	996	MET	2.2
1	A	499	PHE	2.2
1	B	320	LYS	2.2
1	B	1409	ILE	2.2
1	A	296	LYS	2.2
1	A	524	TYR	2.2
1	B	884	THR	2.1
1	A	716	GLU	2.1
1	A	1127	MET	2.1
1	B	1258	TYR	2.1
1	B	50	GLU	2.1
1	B	1222	VAL	2.1
1	B	1201	ASN	2.1
1	A	879	PHE	2.1
1	B	874	LEU	2.1
1	B	163	GLY	2.1
1	B	777	GLU	2.1
1	B	366	GLN	2.1
1	B	145	ASP	2.1
1	A	321	TYR	2.1
1	B	499	PHE	2.1
1	B	241	THR	2.1
1	B	1115	PRO	2.1
1	B	457	GLY	2.0
1	B	1102	ILE	2.0
1	A	140	GLN	2.0
1	B	715	GLN	2.0
1	A	463	ARG	2.0
1	B	431	LEU	2.0
1	B	388	GLY	2.0
1	A	364	GLN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.