



Full wwPDB X-ray Structure Validation Report ⓘ

May 10, 2017 – 01:48 PM EDT

PDB ID : 5XA1
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor cytosolic domain with inositol 1,4,5-trisphosphate
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 6.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

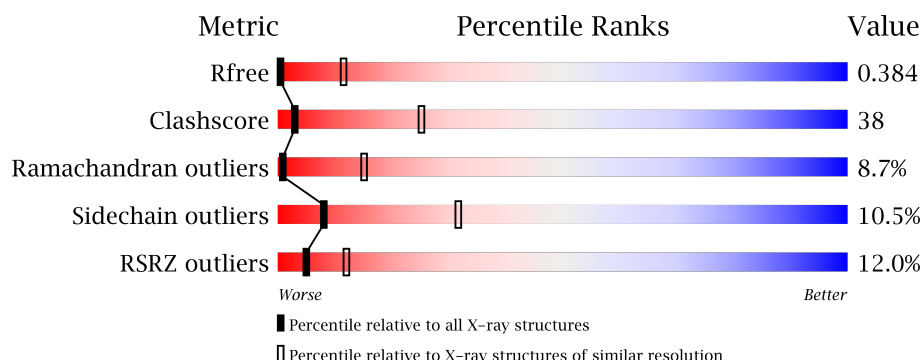
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.20 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	1092 (8.70-3.70)
Clashscore	112137	1023 (8.50-3.80)
Ramachandran outliers	110173	1007 (8.50-3.72)
Sidechain outliers	110143	1091 (8.70-3.70)
RSRZ outliers	101464	1101 (8.70-3.70)

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 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	1581	<div> <div>10%</div> <div>40%</div> <div>33%</div> <div>6%</div> <div>20%</div> </div>
1	B	1581	<div> <div>9%</div> <div>42%</div> <div>32%</div> <div>6%</div> <div>20%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	I3P	A	3000	-	-	-	X
2	I3P	B	3000	-	-	-	X

2 Entry composition [i](#)

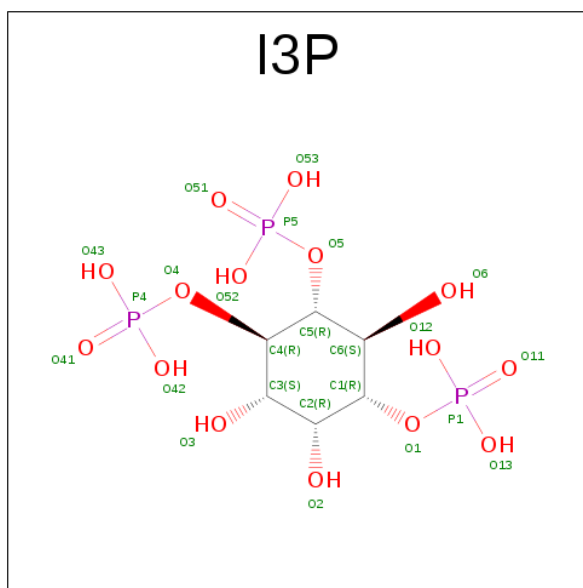
There are 2 unique types of molecules in this entry. The entry contains 25536 atoms, of which 10338 are hydrogens and 0 are deuteriums.

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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1257	Total	C	H	N	O	S	0	0	0
			12735	4648	5160	1435	1475	17			
1	B	1257	Total	C	H	N	O	S	0	0	0
			12735	4648	5160	1435	1475	17			

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).

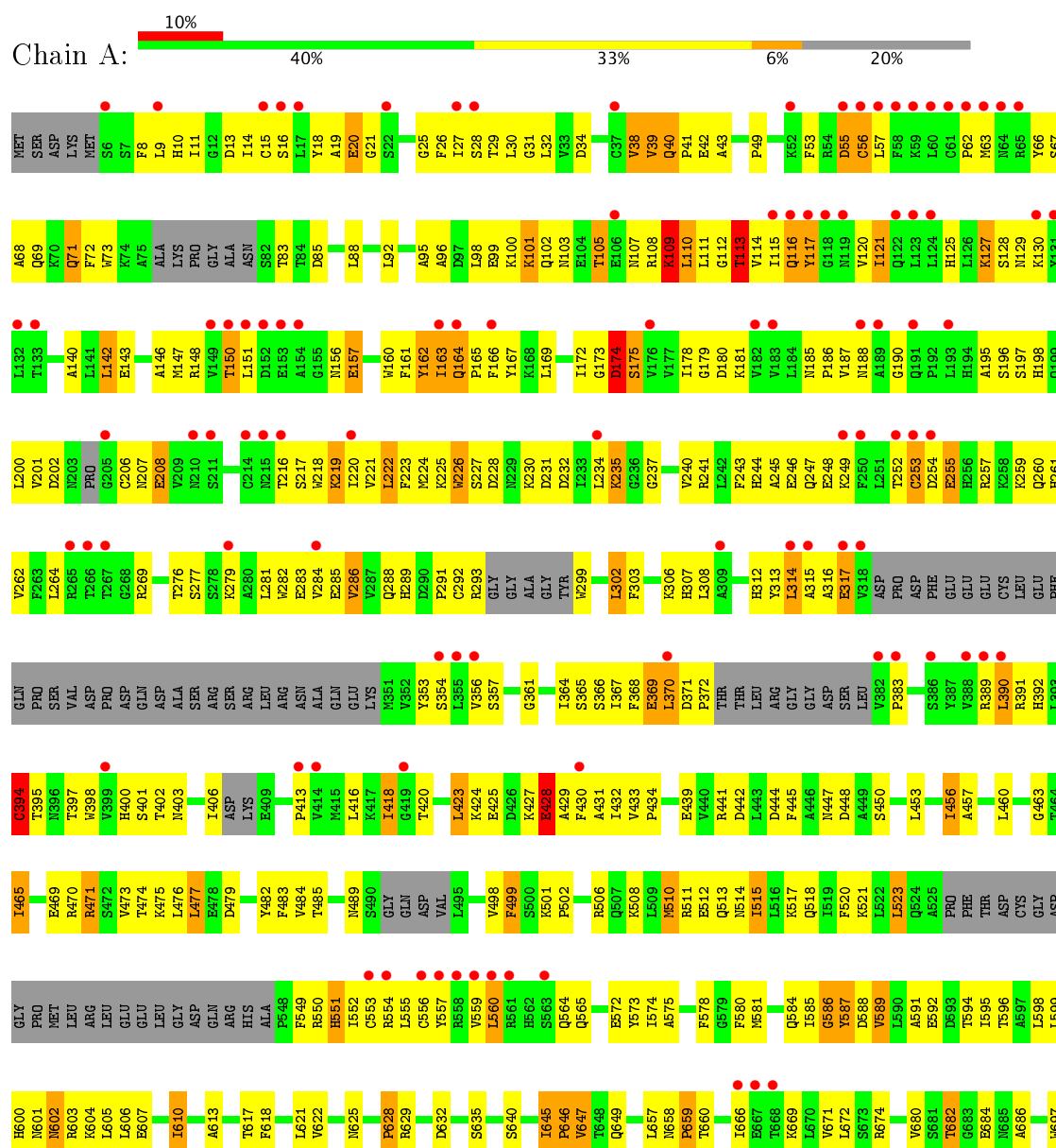


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			33	6	9	15	3		
2	B	1	Total	C	H	O	P	0	0
			33	6	9	15	3		

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: Inositol 1,4,5-trisphosphate receptor type 1





PRO	LEU	Q1081	L993	HIS	K710	R626	C553	T485	K398	PRO	T276	G205	K136
LEU	GLY	F1084	L994	GLY	S711	B627	R564	G486	V399	ASP	S277	G206	R137
HIS	VAL	R1085	L995	THR	R712	R628	C556	N489	T402	GLN	S278	N207	L138
GLU	GLU	H1086	E1000	PRO	R714	R630	L560	S490	L406	ALA	K279	E208	P139
SER	LEU	F1087	S1004	VAL	L715	R632	R561	GLN	ASP	SER	A280	N210	A140
THR	MET	L1088	S1009	LYS	K720	R633	H562	ASP	LYS	ARG	L281	L142	L144
SER	GLN	R1089	S1010	ALA	E721	R634	H563	VAL	E409	SER	E283	E143	E146
VAL	VAL	L1090	S1011	ARG	G722	L636	Q564	L495	LEU	ARG	V284	C214	A146
ASN	VAL	Q1101	S1012	LEU	G723	L637	Q565	L496	E410	LEU	E285	S217	M147
THR	LEU	Q1102	S1013	TRP	D726	C638	D566	L497	E411	ASN	V286	K218	R148
ARG	ARG	D1103	S1014	SER	R727	R639	D567	V497	K412	ALA	V287	W219	V149
VAL	GLY	V1104	S1015	GLU	D728	S640	R568	F499	V413	GLN	Q288	I220	T150
VAL	GLY	Y1112	S1016	ILE	L729	L645	Q571	P502	K414	GLU	H289	V221	L151
GLY	GLY	R1113	S1017	PRO	L730	R646	E572	N503	L416	LYS	D290	L222	D152
ASN	GLY	L1114	S1018	GLU	R731	R647	E573	R504	K417	LYS	F223	F224	E153
SER	PHE	K1115	S1019	SER	S731	R648	E574	R505	L418	GLY	C292	N224	N156
LEU	LEU	D1116	S1020	GLU	Y735	R649	A575	R506	O419	GLY	R293	K225	E157
GLN	PRO	Q1117	S1021	ILE	Q736	R650	A576	Q507	P422	ALA	G158	W226	G158
GLY	MET	L1118	S1022	ALA	L737	C653	K576	K508	L423	ALA	S357	D228	S159
THR	THR	Q1119	S1023	ASP	R738	R654	Q577	L509	K424	GLY	S358	F161	N160
PRO	PRO	Q1120	S1024	ASP	L739	R655	F578	M510	E425	TYR	P359	D231	Y162
SER	MET	Q1121	S1025	TYR	F740	R656	M581	R511	E426	ASP	W239	Y163	I163
ASN	ALA	L1122	S1026	ASP	A741	R657	R582	E512	E427	THR	N360	K235	Q164
ALA	ALA	T1123	S1027	SER	R742	R658	G586	Q513	A429	THR	S301	G236	P165
VAL	PRO	V1124	S1028	SER	L743	R659	Y587	M514	F430	LEU	L302	G237	F166
GLY	GLY	Y1125	S1029	THR	R744	R660	Y588	I515	A431	GLY	F303	D238	Y167
GLY	GLY	Q1126	S1030	THR	A751	D663	V589	L523	I432	ASP	R304	V239	K168
GLY	GLY	L1127	S1031	THR	R752	L664	L590	Q524	V433	ASP	K306	V240	L169
GLY	GLY	Q1128	S1032	THR	E754	L665	A591	A525	V434	ASP	H307	R241	R170
GLY	GLY	Q1129	S1033	THR	L755	L666	E592	PHE	V435	ASP	L308	L242	S175
GLY	GLY	Q1130	S1034	THR	R756	L667	E593	THR	S436	ASP	A309	F243	V176
GLY	GLY	Q1131	S1035	THR	Q758	R668	T594	THR	A437	THR	T310	H244	V177
GLY	GLY	Q1132	S1036	THR	D760	R669	L598	ASP	A438	THR	H312	Q247	L178
GLY	GLY	Q1133	S1037	THR	R761	L670	L599	CYS	D442	LEU	Y313	E248	G179
GLY	GLY	Q1134	S1038	THR	D762	L671	L599	GLY	L443	ARG	L314	K249	D180
GLY	GLY	Q1135	S1039	THR	R763	L672	L599	GLY	D444	GLY	A315	K181	V182
GLY	GLY	Q1136	S1040	THR	S769	R675	M602	GLY	F445	GLY	A316	L251	L183
GLY	GLY	Q1137	S1041	THR	R772	R676	K604	PRO	R446	GLY	E317	T252	L184
GLY	GLY	Q1138	S1042	THR	L773	R677	E607	LEU	A447	SER	G253	D254	N185
GLY	GLY	Q1139	S1043	THR	P774	R678	H609	ARG	D448	LEU	ASP	E255	P186
GLY	GLY	Q1140	S1044	THR	R775	R679	I610	GLY	A449	LEU	PRO	K258	V187
GLY	GLY	Q1141	S1045	THR	L776	R680	T611	GLY	S450	ASP	PHE	N188	A189
GLY	GLY	Q1142	S1046	THR	R777	R681	A612	GLY	R451	GLY	GLY	H261	L193
GLY	GLY	Q1143	S1047	THR	A778	R682	A613	GLY	T456	GLY	CYS	V282	H194
GLY	GLY	Q1144	S1048	THR	S780	R683	D616	GLY	R470	GLY	LEU	L264	A195
GLY	GLY	Q1145	S1049	THR	H787	R684	T617	GLY	R471	GLY	GLY	R265	S196
GLY	GLY	Q1146	S1050	THR	M788	R685	F618	GLY	S472	GLY	PHE	T266	S197
GLY	GLY	Q1147	S1051	THR	H789	R686	V619	HIS	V473	GLY	GLN	Q270	L200
GLY	GLY	Q1148	S1052	THR	D790	R687	S620	ALA	V474	GLY	PRO	S271	N201
GLY	GLY	Q1149	S1053	THR	R791	R688	L621	ALA	V475	GLY	VAL	A272	D202
GLY	GLY	Q1150	S1054	THR	S703	R689	V622	ALA	V476	GLY	ASP	T273	N203
GLY	GLY	Q1151	S1055	THR	ARG	R690	R623	ALA	V477	GLY	PRO	Q271	L201
GLY	GLY	Q1152	S1056	THR	ASP	R691	R624	ALA	V478	GLY	VAL	A273	D202
GLY	GLY	Q1153	S1057	THR	PRO	R692	R625	ALA	V479	GLY	ASP	T274	N203
GLY	GLY	Q1154	S1058	THR	GLN	R693	R626	ALA	V480	GLY	ASP	T275	N204
GLY	GLY	Q1155	S1059	THR	GLY	R694	R627	ALA	V481	GLY	ASP	T276	N205
GLY	GLY	Q1156	S1060	THR	R695	R695	R628	ALA	V482	GLY	ASP	T277	N206
GLY	GLY	Q1157	S1061	THR	R696	R696	R629	ALA	V483	GLY	ASP	T278	N207
GLY	GLY	Q1158	S1062	THR	R697	R697	R630	ALA	V484	GLY	ASP	T279	N208
GLY	GLY	Q1159	S1063	THR	R698	R698	R631	ALA	V485	GLY	ASP	T280	N209
GLY	GLY	Q1160	S1064	THR	R699	R699	R632	ALA	V486	GLY	ASP	T281	N210
GLY	GLY	Q1161	S1065	THR	R700	R700	R633	ALA	V487	GLY	ASP	T282	N211
GLY	GLY	Q1162	S1066	THR	R701	R701	R634	ALA	V488	GLY	ASP	T283	N212
GLY	GLY	Q1163	S1067	THR	D702	R702	R635	ALA	V489	GLY	ASP	T284	N213
GLY	GLY	Q1164	S1068	THR	S703	R703	R636	ALA	V490	GLY	ASP	T285	N214
GLY	GLY	Q1165	S1069	THR	ARG	R704	R637	ALA	V491	GLY	ASP	T286	N215
GLY	GLY	Q1166	S1070	THR	ASP	R705	R638	ALA	V492	GLY	ASP	T287	N216
GLY	GLY	Q1167	S1071	THR	PRO	R706	R639	ALA	V493	GLY	ASP	T288	N217
GLY	GLY	Q1168	S1072	THR	GLN	R707	R640	ALA	V494	GLY	ASP	T289	N218
GLY	GLY	Q1169	S1073	THR	GLY	R708	R641	ALA	V495	GLY	ASP	T290	N219
GLY	GLY	Q1170	S1074	THR	GLY	R709	R642	ALA	V496	GLY	ASP	T291	N220
GLY	GLY	Q1171	S1075	THR	GLY	R710	R643	ALA	V497	GLY	ASP	T292	N221
GLY	GLY	Q1172	S1076	THR	GLY	R711	R644	ALA	V498	GLY	ASP	T293	N222
GLY	GLY	Q1173	S1077	THR	GLY	R712	R645	ALA	V499	GLY	ASP	T294	N223
GLY	GLY	Q1174	S1078	THR	GLY	R713	R646	ALA	V500	GLY	ASP	T295	N224
GLY	GLY	Q1175	S1079	THR	GLY	R714	R647	ALA	V501	GLY	ASP	T296	N225
GLY	GLY	Q1176	S1080	THR	GLY	R715	R648	ALA	V502	GLY	ASP	T297	N226
GLY	GLY	Q1177	S1081	THR	GLY	R716	R649	ALA	V503	GLY	ASP	T298	N227
GLY	GLY	Q1178	S1082	THR	GLY	R717	R650	ALA	V504	GLY	ASP	T299	N228
GLY	GLY	Q1179	S1083	THR	GLY	R718	R651	ALA	V505	GLY	ASP	T300	N229
GLY	GLY	Q1180	S1084	THR	GLY	R719	R652	ALA	V506	GLY	ASP	T301	N230
GLY	GLY	Q1181	S1085	THR	GLY	R720	R653	ALA	V507	GLY	ASP	T302	N231
GLY	GLY	Q1182	S1086	THR	GLY	R721	R654	ALA	V508	GLY	ASP	T303	N232
GLY	GLY	Q1183	S1087	THR	GLY	R722	R655	ALA	V509	GLY	ASP	T304	N233
GLY	GLY	Q1184	S1088	THR	GLY	R723	R656	ALA	V510	GLY	ASP	T305	N234
GLY	GLY	Q1185	S1089	THR	GLY	R724	R657	ALA	V511	GLY	ASP	T306	N235
GLY	GLY	Q1186	S1090	THR	GLY	R725	R658	ALA	V512	GLY	ASP	T307	N236
GLY	GLY	Q1187	S1091	THR	GLY	R726	R659	ALA	V513	GLY	ASP	T308	N237
GLY	GLY	Q1188	S1092	THR	GLY	R727	R660	ALA	V514	GLY	ASP	T309	N238
GLY	GLY	Q1189	S1093	THR	GLY	R728	R661	ALA	V515	GLY	ASP	T310	N239
GLY	GLY	Q1190	S1094	THR	GLY	R729	R662	ALA	V516	GLY	ASP	T311	N240
GLY	GLY	Q1191	S1095	THR	GLY	R730	R663	ALA	V517	GLY	ASP	T312	N241
GLY	GLY	Q1192	S1096	THR	GLY	R731	R664	ALA	V518	GLY	ASP	T313	N242
GLY	GLY	Q1193	S1097	THR	GLY	R732	R665	ALA	V519	GLY	ASP	T314	N243
GLY	GLY	Q1194	S1098	THR	GLY	R733	R666	ALA	V520	GLY	ASP	T315	N244
GLY	GLY	Q1195	S1099	THR	GLY	R734	R667	ALA	V521	GLY	ASP	T316	N245
GLY	GLY	Q1196	S1100	THR	GLY	R735	R668	ALA	V522	GLY	ASP	T317	N246
GLY	GLY	Q1197	S1101	THR	GLY	R736	R669	ALA	V523	GLY	ASP	T318	N247
GLY	GLY	Q1198	S1102	THR	GLY	R737	R670	ALA	V524	GLY	ASP	T319	N248
GLY	GLY	Q1199	S1103	THR	GLY	R738	R671	ALA	V525	GLY	ASP	T320	N249
GLY	GLY	Q1200	S1104	THR	GLY	R739	R672	ALA	V526	GLY	ASP	T321	N250
GLY	GLY	Q1201	S1105	THR	GLY	R740	R673	ALA	V527	GLY	ASP	T322	N251
GLY	GLY	Q1202	S1106	THR	GLY	R741	R674	ALA	V528	GLY	ASP	T323	N252
GLY	GLY	Q1203	S1107	THR	GLY	R742	R675	ALA	V529	GLY	ASP	T324	N253
GLY	GLY	Q1204	S1108	THR	GLY	R743	R676	ALA	V530	GLY	ASP	T325	N254
GLY	GLY	Q1205	S1109	THR	GLY	R744	R677	ALA	V531	GLY	ASP	T326	N255
GLY	GLY	Q1206	S1110	THR	GLY	R745	R678	ALA	V532	GLY	ASP	T327	N256
GLY	GLY	Q1207	S1111	THR	GLY	R746	R679	ALA	V533	GLY	ASP	T328	N257
GLY	GLY	Q1208	S1112	THR	GLY	R747	R680	ALA	V534	GLY	ASP	T329	N258



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	126.80Å 126.80Å 367.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 6.20 48.54 – 6.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.50-6.20) 99.6 (48.54-6.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.360 , 0.382 0.362 , 0.384	Depositor DCC
R_{free} test set	650 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 473.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-l	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	25536	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I3P

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	0.91	19/7637 (0.2%)	1.01	27/10494 (0.3%)
1	B	0.80	10/7637 (0.1%)	0.91	8/10494 (0.1%)
All	All	0.86	29/15274 (0.2%)	0.96	35/20988 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	7
All	All	0	17

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	GLN	CB-CG	12.62	1.86	1.52
1	B	1491	SER	C-N	11.74	1.61	1.34
1	A	109	LYS	CB-CG	10.84	1.81	1.52
1	A	116	GLN	CG-CD	9.81	1.73	1.51
1	A	56	CYS	CB-SG	9.68	1.98	1.82
1	A	285	GLU	CA-CB	-8.99	1.34	1.53
1	A	109	LYS	CD-CE	8.79	1.73	1.51
1	B	285	GLU	CA-CB	8.60	1.72	1.53
1	A	428	GLU	CB-CG	-8.10	1.36	1.52
1	A	109	LYS	CG-CD	7.55	1.78	1.52
1	A	208	GLU	CG-CD	-7.24	1.41	1.51
1	A	55	ASP	CB-CG	-6.80	1.37	1.51
1	B	382	VAL	C-N	6.75	1.47	1.34
1	A	1393	GLU	N-CA	6.21	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	GLU	CB-CG	-6.02	1.40	1.52
1	A	303	PHE	CB-CG	5.97	1.61	1.51
1	B	42	GLU	CB-CG	5.93	1.63	1.52
1	A	283	GLU	CB-CG	5.85	1.63	1.52
1	B	20	GLU	CB-CG	-5.61	1.41	1.52
1	A	175	SER	N-CA	5.50	1.57	1.46
1	A	219	LYS	CB-CG	-5.43	1.37	1.52
1	B	439	GLU	CG-CD	-5.43	1.43	1.51
1	A	369	GLU	CG-CD	-5.39	1.43	1.51
1	B	99	GLU	CG-CD	-5.27	1.44	1.51
1	B	505	GLU	CG-CD	5.24	1.59	1.51
1	B	20	GLU	CG-CD	-5.22	1.44	1.51
1	A	157	GLU	CB-CG	5.18	1.61	1.52
1	A	279	LYS	CB-CG	5.05	1.66	1.52
1	B	119	ASN	CB-CG	5.00	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	CYS	CA-CB-SG	9.02	130.24	114.00
1	A	1393	GLU	C-N-CA	8.16	142.11	121.70
1	B	390	LEU	CA-CB-CG	7.72	133.07	115.30
1	A	1395	LYS	CB-CA-C	-7.40	95.59	110.40
1	A	116	GLN	CB-CA-C	7.34	125.08	110.40
1	A	116	GLN	CB-CG-CD	6.88	129.49	111.60
1	B	869	LEU	O-C-N	6.82	133.61	122.70
1	A	253	CYS	CA-CB-SG	6.78	126.20	114.00
1	B	132	LEU	CA-CB-CG	6.70	130.70	115.30
1	A	113	THR	CA-CB-CG2	-6.62	103.13	112.40
1	A	109	LYS	CB-CG-CD	6.62	128.80	111.60
1	A	175	SER	CA-CB-OG	6.32	128.27	111.20
1	B	214	CYS	CA-CB-SG	6.28	125.31	114.00
1	A	390	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	1395	LYS	N-CA-CB	6.18	121.72	110.60
1	A	109	LYS	CG-CD-CE	6.17	130.40	111.90
1	A	477	LEU	CB-CG-CD1	-6.13	100.57	111.00
1	B	869	LEU	CA-C-O	-5.96	107.59	120.10
1	A	1287	ILE	C-N-CA	5.90	136.45	121.70
1	A	314	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	1393	GLU	O-C-N	-5.87	113.31	122.70
1	A	109	LYS	CA-CB-CG	5.86	126.30	113.40
1	A	162	TYR	CA-CB-CG	5.73	124.29	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASP	CA-C-N	5.58	129.48	117.20
1	A	394	CYS	CA-CB-SG	-5.58	103.95	114.00
1	A	1391	TYR	N-CA-CB	-5.51	100.68	110.60
1	A	370	LEU	C-N-CA	5.38	135.15	121.70
1	A	560	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	1393	GLU	CA-C-N	5.31	128.88	117.20
1	A	110	LEU	CB-CG-CD1	5.29	120.00	111.00
1	B	1491	SER	C-N-CA	5.25	134.83	121.70
1	A	116	GLN	N-CA-CB	-5.18	101.28	110.60
1	B	556	CYS	CA-CB-SG	5.13	123.23	114.00
1	B	56	CYS	CA-CB-SG	5.11	123.19	114.00
1	A	510	MET	CA-CB-CG	5.05	121.88	113.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1203	ARG	Peptide
1	A	1228	THR	Peptide
1	A	1342	LEU	Peptide
1	A	1375	ILE	Peptide
1	A	1382	ALA	Peptide
1	A	1393	GLU	Peptide
1	A	173	GLY	Peptide
1	A	174	ASP	Mainchain
1	A	707	ILE	Peptide
1	B	1034	GLU	Peptide
1	B	1375	ILE	Peptide
1	B	1380	LEU	Peptide
1	B	1461	CYS	Peptide
1	B	679	GLY	Peptide
1	B	708	ARG	Peptide
1	B	744	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7575	5160	5277	516	8
1	B	7575	5160	5277	457	0
2	A	24	9	9	0	0
2	B	24	9	9	0	0
All	All	15198	10338	10572	973	8

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 38.

All (973) 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:109:LYS:CG	1:A:109:LYS:CD	1.78	1.61
1:A:109:LYS:CG	1:A:109:LYS:CB	1.81	1.54
1:A:116:GLN:CG	1:A:116:GLN:CB	1.86	1.52
1:B:856:ASP:O	1:B:860:ASN:CB	1.89	1.20
1:A:1214:VAL:O	1:A:1218:LEU:CB	1.92	1.17
1:A:1281:PHE:O	1:A:1285:SER:CB	1.95	1.12
1:B:1116:LYS:O	1:B:1119:LEU:N	1.84	1.09
1:B:1281:PHE:O	1:B:1285:SER:CB	2.03	1.06
1:B:1371:LEU:O	1:B:1375:ILE:N	1.91	1.02
1:A:1371:LEU:O	1:A:1375:ILE:N	1.93	1.01
1:A:1125:ILE:O	1:A:1129:SER:CB	2.09	1.01
1:B:892:LEU:O	1:B:896:ASP:CB	2.10	1.00
1:B:1341:VAL:O	1:B:1345:TYR:N	1.95	0.99
1:A:1422:TYR:O	1:A:1426:LEU:CB	2.12	0.97
1:B:1377:LEU:O	1:B:1381:LEU:CB	2.12	0.97
1:A:705:LYS:HA	1:A:736:GLN:CB	1.94	0.97
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.13	0.97
1:B:654:LYS:O	1:B:658:ASN:N	1.97	0.97
1:B:885:LEU:O	1:B:888:THR:N	1.97	0.96
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.15	0.94
1:B:610:ILE:O	1:B:613:ALA:N	2.01	0.93
1:B:882:SER:O	1:B:885:LEU:N	2.00	0.93
1:B:1118:ASP:O	1:B:1120:ASP:N	2.03	0.91
1:B:840:VAL:O	1:B:843:TYR:N	2.04	0.90
1:A:755:ILE:O	1:A:758:GLN:N	2.03	0.90
1:B:653:CYS:O	1:B:657:LEU:N	2.04	0.90
1:A:885:LEU:O	1:A:888:THR:N	2.06	0.89
1:B:1472:SER:O	1:B:1476:LYS:CB	2.19	0.89
1:B:978:LEU:O	1:B:981:ILE:N	2.05	0.89
1:B:888:THR:O	1:B:891:LEU:N	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.21	0.88
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.21	0.87
1:B:777:LEU:O	1:B:780:SER:N	2.07	0.87
1:A:1381:LEU:HA	1:A:1384:CYS:CB	2.05	0.87
1:A:1459:ARG:O	1:A:1461:CYS:N	2.08	0.86
1:B:1270:ALA:HB2	1:B:1319:GLU:CB	2.05	0.86
1:A:603:ARG:O	1:A:605:LEU:N	2.08	0.85
1:A:1191:SER:CB	1:A:1236:LEU:O	2.25	0.84
1:A:574:ILE:O	1:A:578:PHE:N	2.09	0.84
1:B:285:GLU:O	1:B:287:VAL:N	2.11	0.84
1:B:140:ALA:N	1:B:146:ALA:O	2.09	0.84
1:B:18:TYR:OH	1:B:45:ASP:OD1	1.95	0.83
1:A:1111:ASN:O	1:A:1114:GLN:N	2.12	0.83
1:B:963:GLU:O	1:B:967:VAL:CB	2.27	0.83
1:A:277:SER:OG	1:A:512:GLU:OE1	1.96	0.82
1:B:276:THR:O	1:B:508:LYS:NZ	2.13	0.82
1:B:622:VAL:HA	1:B:631:LEU:CB	2.09	0.82
1:A:703:SER:CB	1:A:710:LYS:CB	2.57	0.82
1:B:624:LYS:O	1:B:626:ARG:N	2.12	0.82
1:B:865:GLU:O	1:B:869:LEU:CB	2.29	0.81
1:B:598:LEU:O	1:B:602:ASN:N	2.13	0.81
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.29	0.81
1:B:1421:ALA:O	1:B:1425:PHE:CB	2.28	0.80
1:B:237:GLY:N	1:B:284:VAL:O	2.15	0.80
1:A:20:GLU:N	1:A:217:SER:O	2.14	0.80
1:A:618:PHE:O	1:A:622:VAL:N	2.15	0.80
1:A:586:GLY:O	1:A:588:ASP:N	2.16	0.79
1:A:49:PRO:HG2	1:A:291:PRO:HG2	1.64	0.79
1:A:595:ILE:O	1:A:598:LEU:CB	2.32	0.79
1:B:1125:ILE:O	1:B:1129:SER:CB	2.30	0.79
1:A:859:LYS:O	1:A:863:THR:CB	2.31	0.78
1:A:15:CYS:SG	1:A:222:LEU:HA	2.23	0.78
1:B:838:GLU:O	1:B:841:GLU:N	2.16	0.78
1:A:140:ALA:N	1:A:146:ALA:O	2.17	0.78
1:A:200:LEU:HD21	1:A:208:GLU:HB2	1.67	0.77
1:B:1049:PRO:O	1:B:1053:ASP:N	2.18	0.77
1:B:1287:ILE:HA	1:B:1344:PHE:CB	2.14	0.77
1:A:1417:GLU:O	1:A:1419:LYS:N	2.17	0.77
1:B:669:LYS:O	1:B:671:VAL:N	2.18	0.77
1:A:1294:HIS:O	1:A:1298:CYS:N	2.17	0.76
1:A:755:ILE:O	1:A:759:LEU:N	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HG2	1:B:291:PRO:HG2	1.67	0.76
1:A:595:ILE:O	1:A:599:LEU:N	2.19	0.76
1:A:1121:GLN:O	1:A:1124:SER:N	2.19	0.75
1:A:863:THR:O	1:A:866:VAL:N	2.18	0.75
1:A:20:GLU:O	1:A:217:SER:OG	2.05	0.75
1:B:47:ASN:O	1:B:49:PRO:HD3	1.86	0.75
1:B:885:LEU:O	1:B:888:THR:CB	2.35	0.74
1:B:607:GLU:O	1:B:611:THR:HA	1.87	0.74
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.35	0.74
1:A:707:ILE:CB	1:A:737:LEU:N	2.51	0.73
1:B:1335:VAL:O	1:B:1384:CYS:CB	2.36	0.73
1:B:32:LEU:HD21	1:B:128:SER:HA	1.71	0.73
1:A:1437:MET:O	1:A:1440:ILE:N	2.17	0.73
1:A:1341:VAL:O	1:A:1345:TYR:N	2.19	0.73
1:B:969:ASP:O	1:B:972:LEU:N	2.20	0.73
1:B:1207:ASN:O	1:B:1209:GLY:N	2.22	0.72
1:A:724:LYS:O	1:A:726:ASP:N	2.22	0.72
1:A:601:ASN:O	1:A:603:ARG:N	2.22	0.72
1:A:16:SER:N	1:A:221:VAL:O	2.19	0.72
1:B:29:THR:HG22	1:B:151:LEU:HD11	1.72	0.72
1:A:1134:TYR:O	1:A:1230:MET:N	2.21	0.72
1:A:224:MET:SD	1:A:228:ASP:HB3	2.30	0.72
1:A:581:MET:HA	1:A:591:ALA:HB1	1.72	0.71
1:A:963:GLU:O	1:A:967:VAL:CB	2.36	0.71
1:B:18:TYR:OH	1:B:24:ASN:HB3	1.89	0.71
1:B:857:LYS:O	1:B:861:LYS:CB	2.39	0.70
1:B:874:ILE:O	1:B:878:PHE:CB	2.39	0.70
1:B:1291:VAL:O	1:B:1293:GLN:N	2.24	0.70
1:A:316:ALA:HB3	1:A:392:HIS:ND1	2.06	0.70
1:A:1435:VAL:CB	1:A:1492:SER:CB	2.70	0.70
1:B:1420:ILE:O	1:B:1424:ASN:CB	2.39	0.70
1:A:871:ARG:HA	1:A:980:PHE:CB	2.21	0.70
1:B:885:LEU:O	1:B:888:THR:CA	2.40	0.70
1:A:523:LEU:HD12	1:A:553:CYS:SG	2.32	0.70
1:B:485:THR:HG21	1:B:562:HIS:CE1	2.26	0.70
1:B:128:SER:HB2	1:B:130:LYS:HE3	1.74	0.70
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.22	0.70
1:A:230:LYS:HA	1:A:232:ASP:N	2.06	0.69
1:B:860:ASN:O	1:B:863:THR:N	2.25	0.69
1:A:450:SER:OG	1:A:513:GLN:O	2.09	0.69
1:A:981:ILE:O	1:A:985:ARG:CB	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1291:VAL:O	1:B:1294:HIS:N	2.26	0.69
1:B:1381:LEU:HA	1:B:1384:CYS:CB	2.22	0.69
1:A:756:SER:O	1:A:760:ASP:N	2.26	0.69
1:A:264:LEU:HG	1:A:418:ILE:HD11	1.73	0.69
1:B:301:SER:O	1:B:303:PHE:CE1	2.46	0.69
1:A:1215:LEU:O	1:A:1219:GLN:N	2.23	0.68
1:B:290:ASP:O	1:B:292:CYS:N	2.25	0.68
1:B:483:PHE:O	1:B:506:ARG:NH1	2.26	0.68
1:B:755:ILE:O	1:B:758:GLN:N	2.26	0.68
1:A:162:TYR:HB3	1:A:164:GLN:NE2	2.08	0.68
1:B:367:ILE:O	1:B:367:ILE:HG23	1.91	0.68
1:A:72:PHE:O	1:A:72:PHE:CG	2.47	0.68
1:B:15:CYS:SG	1:B:222:LEU:HA	2.34	0.68
1:A:1096:ALA:O	1:A:1100:VAL:N	2.27	0.68
1:B:29:THR:HG22	1:B:151:LEU:CD1	2.24	0.68
1:B:194:HIS:CE1	1:B:214:CYS:SG	2.87	0.68
1:B:1203:ARG:CB	1:B:1207:ASN:CB	2.72	0.67
1:A:842:GLU:O	1:A:845:ARG:N	2.27	0.67
1:A:960:PRO:O	1:A:961:GLU:CB	2.41	0.67
1:B:1338:GLY:O	1:B:1342:LEU:CB	2.42	0.67
1:B:1449:LEU:O	1:B:1453:PHE:CB	2.42	0.67
1:B:855:SER:O	1:B:859:LYS:CB	2.43	0.67
1:A:55:ASP:OD1	1:A:127:LYS:HD3	1.94	0.67
1:A:610:ILE:O	1:A:613:ALA:HB3	1.95	0.67
1:B:863:THR:O	1:B:866:VAL:N	2.28	0.67
1:B:39:VAL:HG21	1:B:195:ALA:HB1	1.77	0.66
1:B:1380:LEU:O	1:B:1384:CYS:CB	2.43	0.66
1:B:236:GLY:HA2	1:B:286:VAL:H	1.59	0.66
1:A:1472:SER:O	1:A:1476:LYS:CB	2.43	0.66
1:A:469:GLU:O	1:A:473:VAL:HG23	1.96	0.66
1:A:1285:SER:O	1:A:1341:VAL:CB	2.44	0.66
1:A:243:PHE:O	1:A:430:PHE:HA	1.94	0.66
1:B:313:TYR:CD2	1:B:361:GLY:HA3	2.30	0.66
1:A:29:THR:HG22	1:A:151:LEU:CD1	2.26	0.66
1:A:1251:ASN:CB	1:A:1283:LEU:O	2.44	0.66
1:B:510:MET:HA	1:B:515:ILE:HG13	1.78	0.65
1:B:138:LEU:O	1:B:147:MET:HA	1.97	0.65
1:A:703:SER:O	1:A:733:TYR:HA	1.97	0.65
1:A:477:LEU:O	1:A:555:LEU:HD21	1.97	0.65
1:A:1187:CYS:O	1:A:1191:SER:CB	2.45	0.65
1:A:117:TYR:CZ	1:A:165:PRO:HB3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD21	1:A:128:SER:HA	1.79	0.64
1:A:581:MET:CA	1:A:591:ALA:HB1	2.26	0.64
1:B:31:GLY:HA3	1:B:448:ASP:OD2	1.96	0.64
1:B:726:ASP:O	1:B:729:ILE:N	2.30	0.64
1:A:196:SER:HB2	1:A:208:GLU:O	1.96	0.64
1:A:885:LEU:O	1:A:888:THR:CB	2.46	0.64
1:A:584:GLN:O	1:A:588:ASP:O	2.15	0.64
1:B:769:SER:CB	1:B:779:ALA:HA	2.28	0.64
1:A:117:TYR:O	1:A:172:ILE:HG12	1.97	0.64
1:B:439:GLU:HA	1:B:442:ASP:OD2	1.96	0.64
1:B:891:LEU:O	1:B:895:LEU:CB	2.46	0.64
1:A:162:TYR:CE2	1:A:187:VAL:HA	2.33	0.64
1:A:20:GLU:HB2	1:A:217:SER:O	1.97	0.64
1:A:1417:GLU:O	1:A:1420:ILE:N	2.31	0.64
1:A:871:ARG:CB	1:A:980:PHE:CA	2.75	0.64
1:B:252:THR:OG1	1:B:265:ARG:HB2	1.98	0.63
1:B:65:ARG:N	1:B:103:ASN:OD1	2.31	0.63
1:B:130:LYS:HD2	1:B:151:LEU:HB3	1.81	0.63
1:B:224:MET:SD	1:B:228:ASP:HB3	2.39	0.63
1:B:617:THR:O	1:B:621:LEU:CB	2.46	0.63
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.47	0.63
1:B:852:PHE:O	1:B:856:ASP:N	2.26	0.63
1:A:1245:CYS:CB	1:A:1285:SER:O	2.46	0.63
1:A:261:HIS:ND1	1:A:406:ILE:HD13	2.14	0.63
1:A:240:VAL:HG12	1:A:434:PRO:HA	1.79	0.63
1:B:32:LEU:CD2	1:B:128:SER:HA	2.28	0.63
1:B:1315:ILE:O	1:B:1319:GLU:CB	2.47	0.63
1:A:397:THR:HB	1:A:420:THR:OG1	1.99	0.63
1:A:744:CYS:HA	1:A:1077:SER:CB	2.28	0.63
1:B:1126:VAL:O	1:B:1130:GLU:CB	2.46	0.63
1:B:241:ARG:HG2	1:B:280:ALA:O	1.99	0.63
1:B:364:ILE:HG22	1:B:394:CYS:SG	2.39	0.62
1:A:1335:VAL:O	1:A:1384:CYS:CB	2.47	0.62
1:A:671:VAL:O	1:A:674:ARG:N	2.32	0.62
1:A:1459:ARG:C	1:A:1461:CYS:H	2.01	0.62
1:B:1210:ALA:O	1:B:1214:VAL:CB	2.46	0.62
1:A:1344:PHE:O	1:A:1347:ASP:N	2.31	0.62
1:B:313:TYR:CG	1:B:361:GLY:HA3	2.34	0.62
1:A:1381:LEU:O	1:A:1385:THR:CB	2.47	0.62
1:A:230:LYS:HA	1:A:232:ASP:H	1.63	0.62
1:A:701:ARG:CB	1:A:729:ILE:CB	2.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:NE2	1:A:73:TRP:HZ2	1.98	0.62
1:B:1345:TYR:O	1:B:1350:SER:CB	2.47	0.62
1:A:871:ARG:CB	1:A:980:PHE:HA	2.30	0.62
1:A:705:LYS:C	1:A:707:ILE:H	2.03	0.62
1:B:1085:ARG:C	1:B:1087:PHE:H	2.02	0.62
1:A:244:HIS:CE1	1:A:428:GLU:HA	2.35	0.62
1:A:398:TRP:CZ2	1:A:424:LYS:HD2	2.35	0.61
1:B:367:ILE:O	1:B:367:ILE:CG2	2.49	0.61
1:B:755:ILE:O	1:B:759:LEU:N	2.32	0.61
1:A:253:CYS:HB2	1:A:307:HIS:CE1	2.36	0.61
1:B:1118:ASP:O	1:B:1121:GLN:N	2.34	0.61
1:B:116:GLN:HA	1:B:175:SER:HA	1.81	0.61
1:B:240:VAL:HG12	1:B:434:PRO:HA	1.81	0.61
1:A:701:ARG:O	1:A:703:SER:N	2.33	0.61
1:A:769:SER:CB	1:A:779:ALA:HA	2.30	0.61
1:A:863:THR:O	1:A:864:PHE:C	2.37	0.61
1:B:313:TYR:CE2	1:B:361:GLY:HA3	2.35	0.61
1:A:761:VAL:O	1:A:764:ILE:N	2.27	0.61
1:B:1118:ASP:O	1:B:1119:LEU:C	2.39	0.61
1:B:134:VAL:HG21	1:B:186:PRO:HG3	1.81	0.61
1:A:1273:MET:O	1:A:1276:ILE:N	2.33	0.61
1:A:243:PHE:HB3	1:A:431:ALA:HB3	1.82	0.61
1:A:761:VAL:O	1:A:763:LEU:N	2.34	0.61
1:B:982:LEU:O	1:B:986:LEU:CB	2.49	0.61
1:A:581:MET:O	1:A:585:ILE:N	2.34	0.60
1:B:117:TYR:OH	1:B:180:ASP:OD2	2.13	0.60
1:A:245:ALA:N	1:A:429:ALA:O	2.34	0.60
1:A:755:ILE:O	1:A:758:GLN:CA	2.49	0.60
1:B:1374:HIS:HA	1:B:1377:LEU:CB	2.32	0.60
1:B:369:GLU:HG2	1:B:370:LEU:N	2.17	0.60
1:B:751:ALA:O	1:B:754:GLU:N	2.34	0.60
1:A:1471:ASP:O	1:A:1474:LEU:N	2.34	0.60
1:A:281:LEU:O	1:A:308:LEU:CB	2.49	0.60
1:A:20:GLU:OE1	1:A:181:LYS:HD3	2.01	0.60
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.35	0.60
1:B:594:THR:O	1:B:598:LEU:N	2.34	0.60
1:A:196:SER:CB	1:A:208:GLU:O	2.50	0.60
1:A:224:MET:HA	1:A:293:ARG:CB	2.32	0.60
1:A:470:ARG:HD2	1:A:471:ARG:HH21	1.65	0.60
1:A:841:GLU:O	1:A:844:LEU:N	2.34	0.60
1:B:36:ARG:NH1	1:B:200:LEU:HD13	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:VAL:O	1:B:640:SER:CB	2.49	0.60
1:B:1215:LEU:O	1:B:1217:LEU:N	2.35	0.60
1:A:728:ASP:CB	1:A:865:GLU:O	2.50	0.59
1:A:15:CYS:CB	1:A:222:LEU:HA	2.32	0.59
1:A:249:LYS:O	1:A:264:LEU:HD22	2.02	0.59
1:A:16:SER:O	1:A:221:VAL:N	2.23	0.59
1:B:134:VAL:N	1:B:158:GLY:O	2.35	0.59
1:A:1203:ARG:CB	1:A:1207:ASN:CB	2.80	0.59
1:B:243:PHE:HB3	1:B:431:ALA:HB3	1.84	0.59
1:A:31:GLY:HA3	1:A:448:ASP:OD2	2.02	0.59
1:B:1405:ILE:O	1:B:1408:VAL:N	2.36	0.59
1:A:1310:LYS:O	1:A:1311:PHE:CB	2.50	0.59
1:A:423:LEU:HD22	1:A:425:GLU:OE1	2.02	0.59
1:B:264:LEU:HG	1:B:418:ILE:HD11	1.85	0.59
1:A:11:ILE:O	1:A:112:GLY:N	2.35	0.59
1:A:456:ILE:HG12	1:A:473:VAL:HG21	1.84	0.59
1:A:313:TYR:CD2	1:A:361:GLY:HA3	2.37	0.59
1:A:439:GLU:HA	1:A:442:ASP:OD2	2.03	0.59
1:B:1317:LYS:HA	1:B:1323:ILE:CB	2.33	0.59
1:A:477:LEU:HB3	1:A:555:LEU:HD22	1.84	0.58
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.33	0.58
1:A:1438:LYS:O	1:A:1441:TYR:N	2.36	0.58
1:A:20:GLU:OE2	1:A:181:LYS:NZ	2.34	0.58
1:A:313:TYR:CG	1:A:361:GLY:HA3	2.38	0.58
1:A:836:THR:O	1:A:839:PHE:N	2.36	0.58
1:B:1000:GLU:CB	1:B:1004:SER:O	2.51	0.58
1:B:54:ARG:CZ	1:B:127:LYS:HG3	2.32	0.58
1:A:1200:GLN:O	1:A:1201:GLN:C	2.41	0.58
1:A:839:PHE:O	1:A:842:GLU:CB	2.51	0.58
1:B:852:PHE:O	1:B:853:PRO:O	2.22	0.58
1:B:1200:GLN:O	1:B:1202:GLN:N	2.36	0.58
1:B:592:GLU:O	1:B:594:THR:N	2.36	0.58
1:A:1203:ARG:O	1:A:1207:ASN:N	2.37	0.58
1:A:1203:ARG:O	1:A:1207:ASN:CB	2.51	0.58
1:A:398:TRP:CD2	1:A:424:LYS:HG3	2.38	0.58
1:B:313:TYR:CD1	1:B:361:GLY:HA3	2.38	0.58
1:A:220:ILE:HG23	1:A:220:ILE:O	2.03	0.58
1:B:225:LYS:C	1:B:227:SER:H	2.06	0.58
1:A:600:HIS:O	1:A:603:ARG:CB	2.52	0.58
1:A:282:TRP:CH2	1:A:314:LEU:HD22	2.39	0.58
1:B:1298:CYS:O	1:B:1299:ILE:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:GLN:O	1:B:574:ILE:N	2.36	0.58
1:A:142:LEU:HB2	1:A:208:GLU:CD	2.24	0.57
1:B:1379:GLU:HA	1:B:1382:ALA:HB3	1.86	0.57
1:B:286:VAL:O	1:B:288:GLN:HG2	2.04	0.57
1:A:489:ASN:OD1	1:A:499:PHE:O	2.23	0.57
1:A:1074:PRO:C	1:A:1076:VAL:H	2.07	0.57
1:A:1210:ALA:O	1:A:1214:VAL:CB	2.53	0.57
1:A:1188:VAL:HA	1:A:1236:LEU:CB	2.34	0.57
1:B:450:SER:OG	1:B:513:GLN:O	2.22	0.57
1:A:364:ILE:O	1:A:394:CYS:SG	2.63	0.57
1:A:1375:ILE:HA	1:A:1378:VAL:CB	2.35	0.57
1:A:555:LEU:HD23	1:A:555:LEU:O	2.05	0.57
1:A:246:GLU:HB2	1:A:427:LYS:HB3	1.86	0.57
1:B:1273:MET:O	1:B:1276:ILE:N	2.38	0.57
1:A:761:VAL:O	1:A:762:ASP:C	2.44	0.57
1:B:863:THR:O	1:B:864:PHE:C	2.42	0.57
1:B:1122:LEU:O	1:B:1125:ILE:N	2.38	0.56
1:B:313:TYR:CZ	1:B:361:GLY:HA3	2.40	0.56
1:A:1294:HIS:O	1:A:1298:CYS:CB	2.54	0.56
1:A:264:LEU:HG	1:A:418:ILE:CD1	2.35	0.56
1:A:71:GLN:HB3	1:A:92:LEU:CD2	2.35	0.56
1:B:55:ASP:OD1	1:B:127:LYS:HD3	2.06	0.56
1:A:400:HIS:HA	1:A:428:GLU:HG2	1.87	0.56
1:A:39:VAL:O	1:A:41:PRO:HD3	2.04	0.56
1:A:744:CYS:O	1:A:1077:SER:CB	2.53	0.56
1:B:1108:ASP:O	1:B:1112:TYR:CB	2.53	0.56
1:B:1435:VAL:CB	1:B:1492:SER:CB	2.83	0.56
1:A:767:CYS:O	1:A:771:GLU:CB	2.54	0.56
1:B:616:ASP:O	1:B:620:SER:CB	2.54	0.56
1:A:1207:ASN:O	1:A:1210:ALA:N	2.37	0.56
1:B:20:GLU:OE2	1:B:181:LYS:NZ	2.36	0.56
1:B:64:ASN:HB2	1:B:66:TYR:CE2	2.40	0.56
1:A:1215:LEU:O	1:A:1218:LEU:N	2.39	0.56
1:B:871:ARG:CB	1:B:980:PHE:HA	2.36	0.56
1:B:194:HIS:CD2	1:B:214:CYS:HB2	2.41	0.56
1:B:165:PRO:HB2	1:B:170:ARG:O	2.06	0.56
1:B:20:GLU:HB2	1:B:217:SER:O	2.06	0.56
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.41	0.56
1:A:368:PHE:CD1	1:A:392:HIS:HA	2.41	0.56
1:A:975:ILE:O	1:A:979:GLN:CB	2.54	0.56
1:B:1203:ARG:O	1:B:1207:ASN:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:CA	1:A:980:PHE:CB	2.83	0.55
1:B:1434:GLU:O	1:B:1492:SER:CB	2.55	0.55
1:B:170:ARG:NH2	1:B:180:ASP:OD1	2.38	0.55
1:B:769:SER:O	1:B:773:LEU:CB	2.54	0.55
1:A:708:ARG:O	1:A:712:VAL:N	2.39	0.55
1:A:1434:GLU:O	1:A:1492:SER:CB	2.54	0.55
1:A:610:ILE:O	1:A:613:ALA:CB	2.53	0.55
1:B:142:LEU:HD21	1:B:200:LEU:HA	1.88	0.55
1:B:30:LEU:HD12	1:B:36:ARG:NH2	2.20	0.55
1:A:1361:GLU:O	1:A:1364:ARG:CB	2.54	0.55
1:B:1245:CYS:CB	1:B:1341:VAL:H	2.20	0.55
1:B:1284:CYS:CB	1:B:1295:PHE:CB	2.85	0.55
1:B:20:GLU:N	1:B:217:SER:O	2.38	0.55
1:B:633:TYR:O	1:B:636:ASP:N	2.40	0.55
1:B:860:ASN:O	1:B:861:LYS:C	2.45	0.55
1:A:312:HIS:CB	1:A:357:SER:OG	2.54	0.55
1:A:66:TYR:O	1:A:157:GLU:OE2	2.23	0.55
1:A:364:ILE:O	1:A:367:ILE:HG22	2.07	0.55
1:A:1200:GLN:C	1:A:1202:GLN:N	2.56	0.55
1:B:1245:CYS:CB	1:B:1285:SER:O	2.55	0.55
1:B:726:ASP:O	1:B:728:ASP:N	2.40	0.55
1:A:142:LEU:HB2	1:A:208:GLU:OE2	2.06	0.55
1:A:181:LYS:HA	1:A:218:TRP:O	2.07	0.55
1:A:671:VAL:O	1:A:674:ARG:CB	2.55	0.55
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.55	0.55
1:B:1245:CYS:CB	1:B:1285:SER:CB	2.84	0.55
1:B:1285:SER:HA	1:B:1341:VAL:CB	2.37	0.55
1:B:136:LYS:HB3	1:B:189:ALA:HA	1.89	0.55
1:A:861:LYS:O	1:A:864:PHE:N	2.40	0.54
1:A:885:LEU:O	1:A:888:THR:CA	2.55	0.54
1:A:844:LEU:HA	1:A:847:VAL:CB	2.38	0.54
1:B:13:ASP:OD1	1:B:226:TRP:N	2.40	0.54
1:B:511:ARG:O	1:B:511:ARG:HG2	2.07	0.54
1:A:244:HIS:CD2	1:A:264:LEU:HD11	2.43	0.54
1:A:788:MET:O	1:A:790:VAL:N	2.41	0.54
1:B:1234:MET:O	1:B:1237:ALA:HB3	2.08	0.54
1:B:389:ARG:CZ	1:B:425:GLU:O	2.55	0.54
1:A:999:ARG:HA	1:A:1007:GLN:HA	1.88	0.54
1:A:223:PHE:CD1	1:A:292:CYS:HA	2.43	0.54
1:B:270:GLN:NE2	1:B:1257:LYS:HA	2.22	0.54
1:B:34:ASP:OD2	1:B:36:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:ILE:O	1:A:1319:GLU:CB	2.56	0.54
1:B:65:ARG:H	1:B:103:ASN:CG	2.11	0.54
1:B:18:TYR:HA	1:B:25:GLY:O	2.08	0.54
1:A:142:LEU:HD21	1:A:200:LEU:HA	1.88	0.54
1:A:142:LEU:HD23	1:A:200:LEU:HD23	1.90	0.54
1:A:20:GLU:OE1	1:A:219:LYS:HB2	2.08	0.54
1:A:39:VAL:HG21	1:A:195:ALA:HB1	1.89	0.54
1:A:477:LEU:O	1:A:555:LEU:CD2	2.56	0.54
1:A:756:SER:HA	1:A:759:LEU:CB	2.37	0.54
1:A:789:HIS:O	1:A:790:VAL:CB	2.56	0.54
1:B:744:CYS:CB	1:B:1081:GLN:O	2.56	0.54
1:B:130:LYS:HB2	1:B:151:LEU:HD22	1.90	0.54
1:A:879:TYR:H	1:A:884:LEU:CB	2.21	0.54
1:B:225:LYS:O	1:B:227:SER:N	2.38	0.54
1:B:270:GLN:HE22	1:B:1257:LYS:HA	1.73	0.54
1:B:836:THR:O	1:B:838:GLU:N	2.41	0.54
1:A:108:ARG:O	1:A:111:LEU:HB2	2.08	0.53
1:A:29:THR:HG22	1:A:151:LEU:HD11	1.90	0.53
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.39	0.53
1:A:257:ARG:O	1:A:259:LYS:HG3	2.08	0.53
1:A:316:ALA:HA	1:A:354:SER:O	2.09	0.53
1:B:19:ALA:O	1:B:24:ASN:HA	2.08	0.53
1:B:14:ILE:HG22	1:B:57:LEU:HD22	1.91	0.53
1:B:313:TYR:CE1	1:B:361:GLY:HA3	2.43	0.53
1:A:10:HIS:HA	1:A:113:THR:O	2.09	0.53
1:A:115:ILE:CG2	1:A:116:GLN:N	2.71	0.53
1:A:196:SER:OG	1:A:197:SER:N	2.41	0.53
1:A:371:ASP:HB3	1:A:389:ARG:O	2.09	0.53
1:A:1207:ASN:O	1:A:1209:GLY:N	2.41	0.53
1:A:707:ILE:CB	1:A:733:TYR:O	2.57	0.53
1:A:871:ARG:HA	1:A:980:PHE:HA	1.89	0.53
1:B:186:PRO:HB2	1:B:189:ALA:HB3	1.91	0.53
1:B:1191:SER:CB	1:B:1236:LEU:O	2.57	0.53
1:B:772:ASN:O	1:B:773:LEU:C	2.46	0.53
1:B:856:ASP:HA	1:B:859:LYS:CB	2.39	0.53
1:B:882:SER:O	1:B:885:LEU:CA	2.56	0.53
1:A:40:GLN:CB	1:A:43:ALA:CB	2.87	0.53
1:A:63:MET:SD	1:A:120:VAL:HG21	2.48	0.53
1:A:867:VAL:CB	1:A:976:GLU:CB	2.87	0.53
1:B:194:HIS:CD2	1:B:214:CYS:CB	2.92	0.53
1:A:38:VAL:HG11	1:A:200:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LEU:HD12	1:B:553:CYS:SG	2.49	0.53
1:A:1201:GLN:O	1:A:1202:GLN:C	2.47	0.52
1:A:353:TYR:O	1:A:420:THR:HG22	2.08	0.52
1:B:484:VAL:HG11	1:B:562:HIS:HB3	1.91	0.52
1:A:142:LEU:HD12	1:A:198:HIS:HB3	1.91	0.52
1:A:225:LYS:O	1:A:227:SER:N	2.39	0.52
1:A:657:LEU:O	1:A:659:PRO:N	2.41	0.52
1:B:669:LYS:C	1:B:671:VAL:N	2.62	0.52
1:A:1438:LYS:HA	1:A:1441:TYR:CB	2.39	0.52
1:A:772:ASN:O	1:A:773:LEU:C	2.48	0.52
1:B:1200:GLN:C	1:B:1202:GLN:N	2.62	0.52
1:A:113:THR:O	1:A:114:VAL:C	2.44	0.52
1:A:369:GLU:OE2	1:A:391:ARG:NH2	2.33	0.52
1:A:581:MET:O	1:A:585:ILE:CB	2.57	0.52
1:B:1476:LYS:O	1:B:1479:THR:N	2.42	0.52
1:B:701:ARG:O	1:B:703:SER:N	2.43	0.52
1:B:1207:ASN:O	1:B:1210:ALA:N	2.43	0.52
1:B:1245:CYS:CB	1:B:1341:VAL:N	2.72	0.52
1:A:15:CYS:HA	1:A:223:PHE:N	2.25	0.52
1:A:299:TRP:CZ2	1:A:372:PRO:HD3	2.45	0.52
1:A:511:ARG:O	1:A:511:ARG:HG2	2.10	0.52
1:A:871:ARG:CB	1:A:980:PHE:N	2.72	0.52
1:B:1116:LYS:O	1:B:1117:GLN:C	2.48	0.52
1:B:124:LEU:HD13	1:B:131:TYR:CE1	2.45	0.52
1:B:69:GLN:HG2	1:B:73:TRP:CZ2	2.45	0.52
1:A:117:TYR:CE2	1:A:165:PRO:HB3	2.43	0.52
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.92	0.52
1:A:753:ASN:O	1:A:754:GLU:C	2.48	0.52
1:B:194:HIS:CG	1:B:214:CYS:HG	2.28	0.52
1:B:830:LYS:O	1:B:833:PHE:CB	2.58	0.52
1:A:447:ASN:O	1:A:448:ASP:C	2.45	0.52
1:A:514:ASN:ND2	1:A:517:LYS:HD3	2.25	0.52
1:B:134:VAL:HG23	1:B:161:PHE:CZ	2.45	0.52
1:B:470:ARG:NH2	1:B:548:PRO:HA	2.25	0.52
1:B:992:CYS:O	1:B:995:CYS:N	2.43	0.52
1:A:772:ASN:O	1:A:774:PRO:N	2.43	0.52
1:B:1064:LEU:CB	1:B:1101:GLN:CB	2.87	0.52
1:B:627:GLU:O	1:B:629:ARG:N	2.43	0.51
1:B:669:LYS:C	1:B:671:VAL:H	2.13	0.51
1:A:727:ARG:O	1:A:730:LEU:N	2.43	0.51
1:B:485:THR:CG2	1:B:562:HIS:ND1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:GLY:O	1:A:1342:LEU:CB	2.59	0.51
1:A:861:LYS:O	1:A:862:LEU:C	2.47	0.51
1:B:1200:GLN:C	1:B:1202:GLN:H	2.14	0.51
1:B:859:LYS:O	1:B:860:ASN:C	2.49	0.51
1:A:1346:ASN:O	1:A:1348:ARG:N	2.44	0.51
1:A:15:CYS:SG	1:A:222:LEU:HG	2.51	0.51
1:A:148:ARG:HG2	1:A:150:THR:HG22	1.93	0.51
1:A:1436:GLU:CB	1:A:1493:PRO:C	2.79	0.51
1:A:14:ILE:O	1:A:222:LEU:HD23	2.10	0.51
1:B:288:GLN:HG3	1:B:292:CYS:O	2.11	0.51
1:B:669:LYS:O	1:B:672:LEU:N	2.43	0.51
1:B:860:ASN:O	1:B:863:THR:CB	2.59	0.51
1:B:888:THR:O	1:B:889:LYS:C	2.49	0.51
1:B:967:VAL:HA	1:B:970:THR:CB	2.40	0.51
1:A:20:GLU:OE2	1:A:181:LYS:CE	2.58	0.51
1:A:460:LEU:HD13	1:A:465:ILE:HG23	1.93	0.51
1:A:843:TYR:O	1:A:847:VAL:CB	2.59	0.51
1:A:998:LYS:CB	1:A:1008:SER:CB	2.89	0.51
1:B:1251:ASN:O	1:B:1255:LEU:CB	2.58	0.51
1:A:140:ALA:HB2	1:A:147:MET:O	2.11	0.51
1:A:66:TYR:CD1	1:A:69:GLN:OE1	2.64	0.51
1:A:697:TRP:CB	1:A:726:ASP:CB	2.89	0.51
1:B:1084:PHE:O	1:B:1087:PHE:CB	2.59	0.51
1:B:196:SER:OG	1:B:197:SER:N	2.44	0.51
1:A:11:ILE:HG21	1:A:62:PRO:HG3	1.93	0.50
1:A:241:ARG:NH2	1:A:439:GLU:OE1	2.42	0.50
1:B:122:GLN:HG2	1:B:159:SER:O	2.10	0.50
1:B:665:LEU:O	1:B:666:ILE:CB	2.59	0.50
1:A:1034:GLU:HA	1:A:1037:ALA:HB3	1.93	0.50
1:A:21:GLY:HA3	1:A:216:THR:HA	1.94	0.50
1:A:398:TRP:CH2	1:A:424:LYS:HE3	2.46	0.50
1:A:473:VAL:O	1:A:476:LEU:N	2.44	0.50
1:A:708:ARG:O	1:A:712:VAL:CB	2.58	0.50
1:A:999:ARG:HA	1:A:1007:GLN:CA	2.40	0.50
1:B:1215:LEU:O	1:B:1218:LEU:N	2.45	0.50
1:A:255:GLU:HA	1:A:259:LYS:O	2.11	0.50
1:A:8:PHE:O	1:A:10:HIS:CE1	2.64	0.50
1:B:1207:ASN:O	1:B:1208:MET:C	2.49	0.50
1:B:609:HIS:O	1:B:610:ILE:C	2.50	0.50
1:A:224:MET:SD	1:A:228:ASP:CB	2.99	0.50
1:A:502:PRO:HG3	1:A:565:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:HIS:CD2	1:B:214:CYS:SG	3.05	0.50
1:B:38:VAL:HG11	1:B:200:LEU:HD11	1.93	0.50
1:A:306:LYS:HB2	1:A:313:TYR:CZ	2.47	0.50
1:A:852:PHE:O	1:A:856:ASP:CB	2.60	0.50
1:A:856:ASP:O	1:A:860:ASN:CB	2.60	0.50
1:B:1061:LEU:O	1:B:1065:LEU:N	2.31	0.50
1:B:711:SER:CB	1:B:737:LEU:CB	2.89	0.50
1:A:1375:ILE:C	1:A:1378:VAL:H	2.15	0.50
1:A:475:LYS:NZ	1:A:479:ASP:OD1	2.42	0.50
1:A:581:MET:HA	1:A:591:ALA:CB	2.39	0.50
1:A:645:ILE:O	1:A:646:PRO:C	2.50	0.50
1:A:730:LEU:O	1:A:733:TYR:N	2.45	0.50
1:B:891:LEU:HA	1:B:894:ILE:H	1.77	0.50
1:A:9:LEU:HD13	1:A:178:ILE:CD1	2.42	0.50
1:A:245:ALA:HB2	1:A:429:ALA:O	2.11	0.50
1:A:353:TYR:HB2	1:A:420:THR:CG2	2.42	0.50
1:A:871:ARG:CA	1:A:980:PHE:HA	2.42	0.50
1:B:1371:LEU:O	1:B:1375:ILE:CA	2.60	0.50
1:B:1375:ILE:HA	1:B:1378:VAL:CB	2.42	0.50
1:B:194:HIS:CG	1:B:214:CYS:SG	3.05	0.50
1:B:36:ARG:HH12	1:B:200:LEU:HD13	1.76	0.50
1:B:313:TYR:CG	1:B:361:GLY:CA	2.94	0.50
1:B:1215:LEU:O	1:B:1216:GLU:C	2.50	0.50
1:B:1357:MET:O	1:B:1359:ARG:N	2.44	0.50
1:B:39:VAL:HG23	1:B:207:ASN:HB2	1.94	0.50
1:B:263:PHE:CE2	1:B:415:MET:HG2	2.46	0.50
1:B:48:ASN:O	1:B:49:PRO:C	2.49	0.50
1:B:127:LYS:O	1:B:127:LYS:HG2	2.12	0.49
1:B:140:ALA:HB3	1:B:143:GLU:O	2.12	0.49
1:B:502:PRO:HG3	1:B:565:GLN:HG2	1.93	0.49
1:B:978:LEU:O	1:B:981:ILE:CA	2.60	0.49
1:A:40:GLN:CB	1:A:43:ALA:HB2	2.42	0.49
1:B:608:LYS:O	1:B:611:THR:CB	2.60	0.49
1:A:554:ARG:CB	1:A:557:TYR:CB	2.91	0.49
1:B:1134:TYR:O	1:B:1230:MET:CB	2.61	0.49
1:B:1382:ALA:HA	1:B:1385:THR:CB	2.42	0.49
1:B:456:ILE:HG12	1:B:473:VAL:HG21	1.94	0.49
1:B:523:LEU:CD1	1:B:553:CYS:SG	3.01	0.49
1:A:632:ASP:O	1:A:635:SER:N	2.45	0.49
1:B:1027:ALA:O	1:B:1029:ASP:N	2.38	0.49
1:B:235:LYS:O	1:B:236:GLY:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LYS:HZ2	1:B:266:THR:HA	1.78	0.49
1:A:103:ASN:O	1:A:107:ASN:ND2	2.46	0.49
1:A:162:TYR:HB3	1:A:164:GLN:CD	2.33	0.49
1:A:753:ASN:O	1:A:755:ILE:N	2.46	0.49
1:B:1310:LYS:O	1:B:1311:PHE:CB	2.61	0.49
1:B:603:ARG:O	1:B:604:LYS:CB	2.61	0.49
1:B:720:LYS:O	1:B:722:GLY:N	2.44	0.49
1:A:125:HIS:O	1:A:129:ASN:HA	2.12	0.49
1:A:977:ILE:C	1:A:979:GLN:H	2.16	0.49
1:B:1085:ARG:C	1:B:1087:PHE:N	2.66	0.49
1:B:354:SER:HA	1:B:419:GLY:HA2	1.95	0.49
1:B:576:LYS:O	1:B:578:PHE:N	2.45	0.49
1:B:836:THR:O	1:B:839:PHE:N	2.46	0.49
1:A:1096:ALA:O	1:A:1097:PHE:C	2.50	0.49
1:A:428:GLU:CA	1:A:428:GLU:OE2	2.58	0.49
1:A:125:HIS:CE1	1:A:127:LYS:HB3	2.48	0.49
1:A:514:ASN:O	1:A:518:GLN:HG2	2.12	0.49
1:A:549:PHE:O	1:A:552:ILE:N	2.45	0.49
1:A:992:CYS:C	1:A:994:LEU:N	2.65	0.49
1:B:140:ALA:HB2	1:B:147:MET:O	2.13	0.49
1:A:841:GLU:O	1:A:844:LEU:CB	2.60	0.48
1:A:96:ALA:O	1:A:100:LYS:HB2	2.13	0.48
1:B:18:TYR:CE1	1:B:25:GLY:CA	2.96	0.48
1:B:391:ARG:HD2	1:B:396:ASN:OD1	2.13	0.48
1:B:242:LEU:HD23	1:B:432:ILE:HD13	1.94	0.48
1:B:654:LYS:O	1:B:657:LEU:C	2.50	0.48
1:A:125:HIS:HE1	1:A:127:LYS:HB3	1.79	0.48
1:A:1416:PRO:O	1:A:1417:GLU:C	2.50	0.48
1:A:735:TYR:O	1:A:738:ASN:O	2.32	0.48
1:B:236:GLY:CA	1:B:286:VAL:H	2.25	0.48
1:A:20:GLU:OE2	1:A:181:LYS:HE2	2.12	0.48
1:A:20:GLU:OE1	1:A:181:LYS:CD	2.61	0.48
1:B:1207:ASN:C	1:B:1209:GLY:N	2.64	0.48
1:B:285:GLU:C	1:B:287:VAL:N	2.66	0.48
1:B:888:THR:O	1:B:890:ILE:N	2.46	0.48
1:A:725:GLU:CB	1:A:865:GLU:CB	2.91	0.48
1:B:188:ASN:OD1	1:B:189:ALA:N	2.46	0.48
1:B:47:ASN:O	1:B:49:PRO:CD	2.58	0.48
1:B:504:ARG:HD2	1:B:567:TYR:CZ	2.49	0.48
1:B:739:LEU:O	1:B:740:PHE:C	2.49	0.48
1:A:254:ASP:O	1:A:260:GLN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LEU:CB	1:A:779:ALA:N	2.77	0.48
1:B:20:GLU:OE1	1:B:219:LYS:HB2	2.13	0.48
1:B:863:THR:O	1:B:865:GLU:N	2.46	0.48
1:B:484:VAL:CG1	1:B:562:HIS:HB3	2.43	0.48
1:A:1076:VAL:O	1:A:1079:ALA:HB3	2.14	0.48
1:A:755:ILE:O	1:A:756:SER:C	2.50	0.48
1:A:759:LEU:O	1:A:760:ASP:O	2.32	0.48
1:B:236:GLY:H	1:B:286:VAL:CB	2.26	0.48
1:B:165:PRO:CB	1:B:170:ARG:O	2.62	0.48
1:B:666:ILE:N	1:B:667:GLU:HA	2.29	0.48
1:A:1189:GLN:C	1:A:1191:SER:H	2.18	0.48
1:A:992:CYS:O	1:A:993:LEU:C	2.51	0.48
1:B:166:PHE:HE1	1:B:167:TYR:CE1	2.32	0.48
1:B:18:TYR:CE1	1:B:25:GLY:N	2.82	0.48
1:B:32:LEU:HD22	1:B:128:SER:HB2	1.96	0.48
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.64	0.47
1:A:703:SER:O	1:A:733:TYR:CA	2.60	0.47
1:B:744:CYS:C	1:B:745:LEU:O	2.51	0.47
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.62	0.47
1:A:179:GLY:H	1:A:220:ILE:HG23	1.79	0.47
1:A:30:LEU:HB2	1:A:34:ASP:OD2	2.14	0.47
1:B:1076:VAL:O	1:B:1079:ALA:HB3	2.14	0.47
1:B:853:PRO:O	1:B:854:PHE:C	2.51	0.47
1:A:20:GLU:HB2	1:A:217:SER:OG	2.14	0.47
1:A:551:HIS:C	1:A:552:ILE:HG13	2.34	0.47
1:A:704:ASN:O	1:A:736:GLN:CB	2.62	0.47
1:A:891:LEU:O	1:A:894:ILE:N	2.45	0.47
1:B:166:PHE:CE1	1:B:167:TYR:CE1	3.02	0.47
1:A:1298:CYS:O	1:A:1299:ILE:CB	2.63	0.47
1:A:39:VAL:HG23	1:A:207:ASN:HB2	1.96	0.47
1:A:671:VAL:O	1:A:672:LEU:C	2.52	0.47
1:A:69:GLN:CD	1:A:73:TRP:HZ2	2.18	0.47
1:B:1417:GLU:O	1:B:1420:ILE:N	2.44	0.47
1:B:1481:ILE:O	1:B:1485:ILE:CB	2.62	0.47
1:A:162:TYR:HB3	1:A:164:GLN:HE22	1.78	0.47
1:A:705:LYS:C	1:A:707:ILE:N	2.67	0.47
1:B:482:TYR:HD1	1:B:489:ASN:O	1.98	0.47
1:A:98:LEU:HD23	1:A:101:LYS:HE2	1.97	0.47
1:A:115:ILE:CG2	1:A:116:GLN:H	2.27	0.47
1:B:883:ASP:O	1:B:887:LEU:CB	2.63	0.47
1:A:286:VAL:O	1:A:288:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:CB	1:A:736:GLN:CB	2.92	0.47
1:A:847:VAL:CB	1:A:897:CYS:O	2.63	0.47
1:B:409:GLU:HG3	1:B:409:GLU:O	2.14	0.47
1:B:64:ASN:CB	1:B:66:TYR:CE2	2.98	0.47
1:A:891:LEU:O	1:A:892:LEU:C	2.53	0.47
1:B:1289:GLU:C	1:B:1291:VAL:H	2.18	0.47
1:A:1078:GLY:O	1:A:1081:GLN:CB	2.63	0.47
1:A:115:ILE:HG22	1:A:116:GLN:N	2.30	0.47
1:B:1061:LEU:O	1:B:1064:LEU:CB	2.62	0.47
1:A:113:THR:O	1:A:115:ILE:N	2.47	0.46
1:A:510:MET:SD	1:A:515:ILE:HG21	2.55	0.46
1:B:1363:ASP:O	1:B:1366:ASP:CB	2.63	0.46
1:A:20:GLU:CB	1:A:217:SER:OG	2.64	0.46
1:A:680:VAL:C	1:A:682:THR:N	2.68	0.46
1:A:69:GLN:HA	1:A:96:ALA:HB2	1.97	0.46
1:A:871:ARG:HA	1:A:980:PHE:CA	2.45	0.46
1:B:470:ARG:HH22	1:B:548:PRO:HA	1.79	0.46
1:B:49:PRO:O	1:B:50:PRO:O	2.34	0.46
1:B:872:ASN:O	1:B:875:TYR:CB	2.63	0.46
1:A:160:TRP:O	1:A:186:PRO:HA	2.16	0.46
1:B:510:MET:SD	1:B:515:ILE:HG21	2.55	0.46
1:B:980:PHE:O	1:B:981:ILE:C	2.53	0.46
1:A:1477:TYR:O	1:A:1481:ILE:CB	2.63	0.46
1:A:596:THR:C	1:A:598:LEU:N	2.66	0.46
1:A:769:SER:O	1:A:773:LEU:CB	2.64	0.46
1:A:162:TYR:HB2	1:A:185:ASN:O	2.15	0.46
1:A:68:ALA:HA	1:A:71:GLN:HB2	1.98	0.46
1:B:1094:LEU:O	1:B:1095:GLN:C	2.54	0.46
1:B:60:LEU:HD13	1:B:123:LEU:HD23	1.96	0.46
1:B:389:ARG:NH2	1:B:425:GLU:H	2.14	0.46
1:B:891:LEU:HA	1:B:894:ILE:CB	2.45	0.46
1:A:40:GLN:CB	1:A:43:ALA:HB3	2.46	0.46
1:A:479:ASP:O	1:A:482:TYR:HB3	2.16	0.46
1:A:72:PHE:O	1:A:72:PHE:CD1	2.69	0.46
1:A:1065:LEU:HA	1:A:1104:VAL:CB	2.46	0.46
1:B:1028:LEU:O	1:B:1031:GLU:N	2.48	0.46
1:B:1034:GLU:HA	1:B:1037:ALA:HB3	1.98	0.46
1:B:231:ASP:OD2	1:B:434:PRO:HG3	2.16	0.46
1:B:32:LEU:CD2	1:B:128:SER:HB2	2.46	0.46
1:B:993:LEU:HA	1:B:996:ILE:CB	2.46	0.46
1:A:581:MET:O	1:A:591:ALA:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:LEU:O	1:A:716:ALA:C	2.54	0.46
1:B:1238:HIS:O	1:B:1240:PHE:N	2.49	0.46
1:B:707:ILE:CB	1:B:736:GLN:CB	2.94	0.46
1:A:1378:VAL:O	1:A:1382:ALA:HB2	2.16	0.45
1:B:139:PRO:O	1:B:148:ARG:HB2	2.16	0.45
1:B:18:TYR:CD1	1:B:25:GLY:C	2.90	0.45
1:B:194:HIS:NE2	1:B:214:CYS:SG	2.89	0.45
1:B:498:VAL:HB	1:B:499:PHE:CD1	2.51	0.45
1:A:1001:PHE:O	1:A:1002:ASP:CB	2.63	0.45
1:B:65:ARG:HH22	1:B:106:GLU:HG2	1.81	0.45
1:B:622:VAL:CA	1:B:631:LEU:CB	2.89	0.45
1:B:315:ALA:HB1	1:B:365:SER:OG	2.16	0.45
1:B:220:ILE:HG23	1:B:220:ILE:O	2.17	0.45
1:B:836:THR:O	1:B:837:MET:C	2.55	0.45
1:A:485:THR:HB	1:A:501:LYS:O	2.17	0.45
1:A:477:LEU:HD11	1:A:556:CYS:SG	2.57	0.45
1:A:751:ALA:O	1:A:752:ILE:C	2.55	0.45
1:A:833:PHE:O	1:A:836:THR:CB	2.65	0.45
1:B:58:PHE:CZ	1:B:125:HIS:CD2	3.05	0.45
1:B:853:PRO:C	1:B:855:SER:N	2.69	0.45
1:A:32:LEU:CD2	1:A:128:SER:HA	2.46	0.45
1:A:121:ILE:HD13	1:A:161:PHE:O	2.16	0.45
1:A:39:VAL:O	1:A:41:PRO:CD	2.65	0.45
1:B:316:ALA:HA	1:B:354:SER:O	2.16	0.45
1:A:769:SER:HA	1:A:773:LEU:CB	2.47	0.45
1:A:85:ASP:HB2	1:A:88:LEU:HB3	1.99	0.45
1:B:1085:ARG:O	1:B:1087:PHE:N	2.50	0.45
1:B:1201:GLN:O	1:B:1203:ARG:N	2.50	0.45
1:B:1457:ILE:O	1:B:1458:CYS:O	2.34	0.45
1:B:395:THR:O	1:B:396:ASN:C	2.55	0.45
1:B:860:ASN:O	1:B:863:THR:CA	2.65	0.45
1:B:889:LYS:O	1:B:892:LEU:CB	2.65	0.45
1:A:245:ALA:CB	1:A:429:ALA:O	2.65	0.45
1:A:977:ILE:O	1:A:979:GLN:N	2.50	0.45
1:A:998:LYS:C	1:A:1007:GLN:HA	2.37	0.45
1:B:124:LEU:CD1	1:B:131:TYR:CE1	3.00	0.45
1:B:1355:ILE:C	1:B:1357:MET:H	2.20	0.45
1:A:67:SER:O	1:A:71:GLN:OE1	2.34	0.45
1:B:315:ALA:CB	1:B:365:SER:O	2.64	0.45
1:A:196:SER:OG	1:A:198:HIS:N	2.39	0.45
1:A:222:LEU:HD21	1:A:224:MET:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:TYR:CZ	1:A:395:THR:HG22	2.52	0.45
1:B:1251:ASN:CB	1:B:1283:LEU:HA	2.47	0.45
1:B:1371:LEU:O	1:B:1372:MET:C	2.55	0.45
1:B:961:GLU:CB	1:B:963:GLU:H	2.30	0.45
1:A:224:MET:HG3	1:A:293:ARG:CB	2.47	0.44
1:B:1201:GLN:O	1:B:1202:GLN:C	2.55	0.44
1:B:143:GLU:HB2	1:B:210:ASN:HD21	1.82	0.44
1:B:143:GLU:HB2	1:B:210:ASN:ND2	2.32	0.44
1:A:589:VAL:O	1:A:592:GLU:CB	2.65	0.44
1:A:596:THR:HA	1:A:599:LEU:CB	2.47	0.44
1:B:1374:HIS:CA	1:B:1377:LEU:CB	2.95	0.44
1:A:1037:ALA:C	1:A:1039:GLY:N	2.70	0.44
1:A:1094:LEU:O	1:A:1095:GLN:C	2.56	0.44
1:A:1381:LEU:C	1:A:1385:THR:H	2.20	0.44
1:A:601:ASN:C	1:A:603:ARG:N	2.70	0.44
1:A:840:VAL:O	1:A:841:GLU:C	2.52	0.44
1:B:1242:GLN:O	1:B:1243:ASN:CB	2.65	0.44
1:B:243:PHE:O	1:B:430:PHE:HA	2.18	0.44
1:B:304:ARG:CB	1:B:366:SER:O	2.65	0.44
1:B:709:SER:O	1:B:713:ARG:CB	2.65	0.44
1:A:1215:LEU:O	1:A:1216:GLU:C	2.56	0.44
1:A:1253:ALA:HA	1:A:1256:HIS:CB	2.48	0.44
1:A:1371:LEU:O	1:A:1372:MET:C	2.56	0.44
1:A:179:GLY:O	1:A:180:ASP:C	2.55	0.44
1:A:453:LEU:O	1:A:457:ALA:HB3	2.17	0.44
1:B:1200:GLN:O	1:B:1201:GLN:C	2.56	0.44
1:B:18:TYR:CZ	1:B:24:ASN:HB3	2.52	0.44
1:B:735:TYR:C	1:B:737:LEU:H	2.21	0.44
1:B:769:SER:HA	1:B:773:LEU:CB	2.48	0.44
1:B:788:MET:O	1:B:790:VAL:N	2.50	0.44
1:A:249:LYS:HB2	1:A:264:LEU:HD13	1.99	0.44
1:A:313:TYR:CD1	1:A:313:TYR:N	2.84	0.44
1:A:457:ALA:HB1	1:A:521:LYS:O	2.17	0.44
1:B:1116:LYS:O	1:B:1119:LEU:CA	2.63	0.44
1:B:484:VAL:HG13	1:B:485:THR:HG23	2.00	0.44
1:B:523:LEU:HD11	1:B:556:CYS:SG	2.58	0.44
1:B:761:VAL:O	1:B:762:ASP:C	2.55	0.44
1:B:831:GLU:O	1:B:832:ARG:C	2.55	0.44
1:B:1371:LEU:O	1:B:1375:ILE:CB	2.65	0.44
1:B:701:ARG:CB	1:B:729:ILE:CB	2.95	0.44
1:A:225:LYS:C	1:A:227:SER:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:O	1:A:249:LYS:HG3	2.17	0.44
1:A:598:LEU:O	1:A:599:LEU:C	2.56	0.44
1:B:299:TRP:HB2	1:B:382:VAL:CB	2.48	0.44
1:B:54:ARG:O	1:B:54:ARG:HG2	2.18	0.44
1:B:588:ASP:C	1:B:590:LEU:H	2.21	0.44
1:B:741:ALA:CB	1:B:876:PHE:HA	2.47	0.44
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.30	0.44
1:A:21:GLY:CA	1:A:216:THR:HA	2.47	0.44
1:A:353:TYR:HB2	1:A:420:THR:HG21	1.99	0.44
1:A:484:VAL:HG13	1:A:485:THR:HG23	2.00	0.44
1:B:507:GLN:HG2	1:B:563:SER:HA	2.00	0.44
1:B:555:LEU:HD23	1:B:555:LEU:O	2.17	0.44
1:B:99:GLU:O	1:B:103:ASN:ND2	2.51	0.44
1:A:264:LEU:CG	1:A:418:ILE:HD11	2.46	0.44
1:A:69:GLN:HG2	1:A:73:TRP:NE1	2.32	0.44
1:A:773:LEU:CB	1:A:779:ALA:H	2.31	0.44
1:B:364:ILE:O	1:B:394:CYS:SG	2.76	0.44
1:A:224:MET:HE2	1:A:293:ARG:O	2.17	0.43
1:A:166:PHE:CD1	1:A:167:TYR:CE2	3.06	0.43
1:A:237:GLY:N	1:A:284:VAL:O	2.48	0.43
1:A:306:LYS:HD2	1:A:313:TYR:OH	2.17	0.43
1:A:317:GLU:N	1:A:354:SER:O	2.51	0.43
1:A:364:ILE:HG22	1:A:394:CYS:SG	2.59	0.43
1:A:581:MET:CB	1:A:591:ALA:HB1	2.47	0.43
1:A:602:ASN:O	1:A:606:LEU:CB	2.66	0.43
1:B:1284:CYS:O	1:B:1292:VAL:CB	2.66	0.43
1:B:451:LYS:HE2	1:B:451:LYS:HA	2.00	0.43
1:A:1362:ARG:O	1:A:1363:ASP:C	2.55	0.43
1:A:142:LEU:CD2	1:A:200:LEU:HD23	2.48	0.43
1:A:498:VAL:HG12	1:A:499:PHE:HD1	1.82	0.43
1:A:57:LEU:HD21	1:A:223:PHE:HB2	2.00	0.43
1:A:707:ILE:CB	1:A:737:LEU:H	2.26	0.43
1:B:32:LEU:CD2	1:B:128:SER:CB	2.96	0.43
1:B:681:SER:O	1:B:682:THR:C	2.57	0.43
1:B:69:GLN:O	1:B:73:TRP:CE2	2.71	0.43
1:A:20:GLU:C	1:A:217:SER:H	2.22	0.43
1:A:621:LEU:O	1:A:625:ASN:CB	2.66	0.43
1:A:682:THR:O	1:A:686:ALA:HB3	2.19	0.43
1:B:1292:VAL:HA	1:B:1295:PHE:CB	2.49	0.43
1:B:271:SER:O	1:B:272:ALA:C	2.56	0.43
1:B:316:ALA:HB2	1:B:355:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:TYR:CD1	1:B:361:GLY:CA	3.00	0.43
1:B:627:GLU:O	1:B:628:PRO:C	2.57	0.43
1:A:549:PHE:O	1:A:551:HIS:N	2.52	0.43
1:B:177:VAL:HG12	1:B:178:ILE:N	2.33	0.43
1:B:484:VAL:O	1:B:484:VAL:HG22	2.19	0.43
1:B:49:PRO:O	1:B:50:PRO:C	2.55	0.43
1:B:826:LYS:O	1:B:828:GLU:N	2.51	0.43
1:B:960:PRO:O	1:B:961:GLU:CB	2.66	0.43
1:A:114:VAL:CG1	1:A:175:SER:HB3	2.49	0.43
1:A:196:SER:HB3	1:A:208:GLU:O	2.18	0.43
1:A:479:ASP:O	1:A:482:TYR:N	2.52	0.43
1:A:483:PHE:O	1:A:506:ARG:NH1	2.48	0.43
1:A:680:VAL:C	1:A:682:THR:H	2.20	0.43
1:A:73:TRP:N	1:A:73:TRP:CD1	2.87	0.43
1:B:1293:GLN:CB	1:B:1345:TYR:O	2.67	0.43
1:B:18:TYR:CE1	1:B:25:GLY:HA2	2.53	0.43
1:B:586:GLY:O	1:B:588:ASP:N	2.52	0.43
1:A:231:ASP:OD2	1:A:434:PRO:HG3	2.19	0.43
1:A:586:GLY:O	1:A:587:TYR:C	2.54	0.43
1:B:133:THR:HG21	1:B:156:ASN:HD21	1.84	0.43
1:B:224:MET:SD	1:B:228:ASP:CB	3.06	0.43
1:B:485:THR:HG21	1:B:562:HIS:ND1	2.33	0.43
1:B:960:PRO:O	1:B:963:GLU:CB	2.67	0.43
1:A:315:ALA:HB1	1:A:365:SER:OG	2.18	0.43
1:A:95:ALA:O	1:A:99:GLU:HB2	2.18	0.43
1:B:38:VAL:CG1	1:B:200:LEU:HD11	2.49	0.43
1:A:701:ARG:O	1:A:703:SER:O	2.36	0.43
1:B:10:HIS:CE1	1:B:114:VAL:HG22	2.53	0.43
1:B:1291:VAL:C	1:B:1293:GLN:N	2.72	0.43
1:B:134:VAL:HB	1:B:189:ALA:CB	2.49	0.43
1:A:15:CYS:HA	1:A:223:PHE:H	1.84	0.43
1:A:18:TYR:HA	1:A:25:GLY:O	2.19	0.43
1:A:402:THR:O	1:A:403:ASN:OD1	2.37	0.43
1:A:69:GLN:O	1:A:73:TRP:CD1	2.71	0.43
1:A:853:PRO:O	1:A:856:ASP:N	2.51	0.43
1:B:978:LEU:O	1:B:979:GLN:C	2.55	0.43
1:A:1000:GLU:CB	1:A:1005:ASN:HA	2.49	0.42
1:A:744:CYS:CB	1:A:1075:LEU:HA	2.48	0.42
1:A:1103:LEU:O	1:A:1105:THR:N	2.52	0.42
1:A:1369:SER:O	1:A:1370:PRO:C	2.56	0.42
1:A:753:ASN:C	1:A:755:ILE:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1285:SER:O	1:B:1341:VAL:CB	2.67	0.42
1:B:1357:MET:O	1:B:1358:MET:C	2.57	0.42
1:A:361:GLY:O	1:A:366:SER:OG	2.36	0.42
1:B:95:ALA:O	1:B:96:ALA:C	2.55	0.42
1:A:316:ALA:HB3	1:A:392:HIS:CE1	2.54	0.42
1:A:499:PHE:HB2	1:A:501:LYS:HZ3	1.84	0.42
1:B:1062:ARG:O	1:B:1066:HIS:N	2.50	0.42
1:B:1215:LEU:C	1:B:1217:LEU:N	2.73	0.42
1:B:1134:TYR:C	1:B:1230:MET:CB	2.87	0.42
1:B:288:GLN:CD	1:B:293:ARG:C	2.78	0.42
1:B:626:ARG:C	1:B:628:PRO:N	2.71	0.42
1:A:1133:VAL:O	1:A:1134:TYR:CB	2.66	0.42
1:A:755:ILE:O	1:A:758:GLN:CB	2.68	0.42
1:B:62:PRO:HB2	1:B:107:ASN:OD1	2.19	0.42
1:A:1122:LEU:HA	1:A:1125:ILE:CB	2.50	0.42
1:A:163:ILE:O	1:A:164:GLN:OE1	2.38	0.42
1:A:188:ASN:O	1:A:190:GLY:N	2.52	0.42
1:A:253:CYS:SG	1:A:262:VAL:HG22	2.60	0.42
1:A:473:VAL:O	1:A:474:THR:C	2.57	0.42
1:A:73:TRP:CZ3	1:A:156:ASN:HB3	2.55	0.42
1:B:143:GLU:CB	1:B:210:ASN:ND2	2.83	0.42
1:B:389:ARG:NE	1:B:425:GLU:O	2.53	0.42
1:A:1344:PHE:C	1:A:1347:ASP:H	2.23	0.42
1:A:520:PHE:CE2	1:A:560:LEU:HD21	2.53	0.42
1:A:863:THR:O	1:A:866:VAL:CB	2.67	0.42
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.20	0.42
1:B:167:TYR:HE2	1:B:181:LYS:HD2	1.85	0.42
1:B:447:ASN:O	1:B:448:ASP:C	2.57	0.42
1:A:398:TRP:CE2	1:A:424:LYS:HD2	2.54	0.42
1:A:595:ILE:C	1:A:598:LEU:CB	2.88	0.42
1:A:69:GLN:CD	1:A:73:TRP:CZ2	2.92	0.42
1:B:179:GLY:H	1:B:220:ILE:HG23	1.84	0.42
1:A:1273:MET:O	1:A:1274:GLN:C	2.58	0.42
1:A:128:SER:HB2	1:A:130:LYS:HE3	2.00	0.42
1:A:1415:ILE:O	1:A:1416:PRO:C	2.58	0.42
1:A:15:CYS:HA	1:A:222:LEU:HA	2.01	0.42
1:B:1224:LYS:CB	1:B:1319:GLU:O	2.68	0.42
1:B:1415:ILE:O	1:B:1416:PRO:C	2.57	0.42
1:B:398:TRP:CD2	1:B:424:LYS:HG3	2.54	0.42
1:B:438:ALA:O	1:B:442:ASP:OD1	2.37	0.42
1:A:38:VAL:CG1	1:A:200:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PHE:CE2	1:B:125:HIS:HB2	2.54	0.42
1:B:239:VAL:HA	1:B:282:TRP:O	2.20	0.42
1:B:391:ARG:HH22	1:B:393:LEU:HD12	1.85	0.42
1:B:261:HIS:CD2	1:B:406:ILE:HD13	2.55	0.42
1:A:200:LEU:HG	1:A:206:CYS:O	2.20	0.42
1:A:580:PHE:O	1:A:581:MET:C	2.57	0.42
1:A:724:LYS:C	1:A:726:ASP:H	2.23	0.42
1:B:270:GLN:OE1	1:B:1257:LYS:HA	2.20	0.42
1:B:1321:LYS:O	1:B:1323:ILE:N	2.43	0.42
1:B:286:VAL:HA	1:B:303:PHE:CD2	2.55	0.42
1:B:314:LEU:O	1:B:315:ALA:HB2	2.20	0.42
1:A:1200:GLN:O	1:A:1202:GLN:N	2.53	0.41
1:A:1354:LEU:O	1:A:1355:ILE:C	2.58	0.41
1:A:594:THR:O	1:A:598:LEU:N	2.50	0.41
1:A:69:GLN:HA	1:A:96:ALA:CB	2.50	0.41
1:B:316:ALA:HA	1:B:355:LEU:HA	2.02	0.41
1:A:1361:GLU:O	1:A:1364:ARG:N	2.52	0.41
1:A:460:LEU:O	1:A:460:LEU:HG	2.20	0.41
1:A:26:PHE:HB3	1:A:56:CYS:SG	2.60	0.41
1:B:485:THR:O	1:B:486:GLY:C	2.57	0.41
1:B:607:GLU:O	1:B:611:THR:CA	2.62	0.41
1:B:687:LEU:O	1:B:688:GLU:C	2.59	0.41
1:B:755:ILE:O	1:B:758:GLN:CA	2.68	0.41
1:A:1253:ALA:O	1:A:1256:HIS:CB	2.69	0.41
1:A:1437:MET:O	1:A:1438:LYS:C	2.57	0.41
1:A:441:ARG:HA	1:A:444:ASP:OD2	2.20	0.41
1:A:460:LEU:HD12	1:A:463:GLY:O	2.21	0.41
1:A:842:GLU:C	1:A:844:LEU:N	2.73	0.41
1:B:571:GLN:C	1:B:574:ILE:H	2.21	0.41
1:B:826:LYS:O	1:B:827:ASP:C	2.58	0.41
1:B:88:LEU:CD2	1:B:92:LEU:HD12	2.51	0.41
1:A:1030:PHE:O	1:A:1033:ILE:N	2.52	0.41
1:A:1083:LEU:O	1:A:1084:PHE:C	2.59	0.41
1:A:15:CYS:O	1:A:57:LEU:CD2	2.69	0.41
1:A:222:LEU:CD2	1:A:224:MET:O	2.68	0.41
1:A:302:LEU:N	1:A:302:LEU:CD1	2.83	0.41
1:B:236:GLY:HA2	1:B:284:VAL:HG12	2.02	0.41
1:B:244:HIS:CD2	1:B:264:LEU:HD11	2.56	0.41
1:B:446:ALA:HB1	1:B:515:ILE:HD11	2.02	0.41
1:B:666:ILE:CB	1:B:669:LYS:N	2.83	0.41
1:A:13:ASP:OD1	1:A:226:TRP:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:THR:O	1:A:621:LEU:CB	2.68	0.41
1:A:727:ARG:O	1:A:728:ASP:C	2.57	0.41
1:B:27:ILE:HG12	1:B:218:TRP:CZ3	2.56	0.41
1:B:484:VAL:HG11	1:B:562:HIS:CB	2.50	0.41
1:B:49:PRO:C	1:B:50:PRO:O	2.57	0.41
1:B:637:LEU:O	1:B:639:VAL:N	2.53	0.41
1:A:10:HIS:HB3	1:A:112:GLY:O	2.21	0.41
1:A:234:LEU:HD13	1:A:432:ILE:HG21	2.02	0.41
1:A:523:LEU:CD1	1:A:553:CYS:SG	3.07	0.41
1:A:756:SER:O	1:A:759:LEU:N	2.54	0.41
1:A:842:GLU:O	1:A:844:LEU:N	2.54	0.41
1:B:1381:LEU:O	1:B:1385:THR:CB	2.69	0.41
1:B:235:LYS:HD3	1:B:235:LYS:HA	1.83	0.41
1:B:675:PHE:O	1:B:679:GLY:N	2.54	0.41
1:B:772:ASN:O	1:B:774:PRO:N	2.53	0.41
1:B:777:LEU:C	1:B:780:SER:H	2.14	0.41
1:A:166:PHE:CE1	1:A:167:TYR:CZ	3.09	0.41
1:A:313:TYR:HD1	1:A:313:TYR:N	2.18	0.41
1:A:841:GLU:O	1:A:844:LEU:CA	2.67	0.41
1:B:136:LYS:O	1:B:147:MET:HG2	2.21	0.41
1:B:619:VAL:O	1:B:623:ARG:CB	2.69	0.41
1:A:1251:ASN:CB	1:A:1283:LEU:CA	2.99	0.41
1:A:1459:ARG:C	1:A:1461:CYS:N	2.66	0.41
1:A:226:TRP:O	1:A:226:TRP:CE3	2.73	0.41
1:A:276:THR:O	1:A:508:LYS:NZ	2.34	0.41
1:B:576:LYS:C	1:B:578:PHE:N	2.74	0.41
1:A:398:TRP:CZ3	1:A:424:LYS:HE3	2.56	0.41
1:A:555:LEU:O	1:A:559:VAL:HG23	2.20	0.41
1:A:560:LEU:O	1:A:564:GLN:HG2	2.21	0.41
1:A:723:GLN:O	1:A:862:LEU:CB	2.68	0.41
1:B:369:GLU:HG2	1:B:370:LEU:H	1.84	0.41
1:B:95:ALA:O	1:B:98:LEU:N	2.53	0.41
1:A:1374:HIS:O	1:A:1377:LEU:CB	2.69	0.41
1:A:647:VAL:O	1:A:649:GLN:N	2.54	0.41
1:A:863:THR:O	1:A:866:VAL:CA	2.69	0.41
1:B:28:SER:O	1:B:37:CYS:HA	2.21	0.41
1:B:444:ASP:C	1:B:446:ALA:H	2.25	0.41
1:B:852:PHE:O	1:B:856:ASP:CB	2.69	0.41
1:A:19:ALA:HB2	1:A:218:TRP:CH2	2.56	0.41
1:A:401:SER:OG	1:A:428:GLU:OE1	2.34	0.41
1:A:853:PRO:O	1:A:854:PHE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:ILE:HA	1:B:710:LYS:CB	2.50	0.41
1:B:69:GLN:NE2	1:B:73:TRP:HZ2	2.18	0.41
1:A:1079:ALA:O	1:A:1081:GLN:N	2.54	0.40
1:A:1436:GLU:O	1:A:1439:GLU:CB	2.69	0.40
1:A:1489:PHE:O	1:A:1490:PHE:C	2.60	0.40
1:A:369:GLU:HG2	1:A:370:LEU:N	2.35	0.40
1:A:510:MET:CE	1:A:515:ILE:HG13	2.51	0.40
1:A:999:ARG:O	1:A:1006:SER:O	2.39	0.40
1:B:1303:GLY:O	1:B:1304:ARG:C	2.59	0.40
1:B:358:VAL:HA	1:B:359:PRO:HD3	1.91	0.40
1:A:1112:TYR:HA	1:A:1115:ILE:CB	2.51	0.40
1:A:1207:ASN:C	1:A:1209:GLY:N	2.73	0.40
1:A:1405:ILE:O	1:A:1406:VAL:C	2.58	0.40
1:A:143:GLU:HG3	1:A:198:HIS:HE1	1.87	0.40
1:A:367:ILE:O	1:A:367:ILE:HG23	2.21	0.40
1:A:403:ASN:HA	1:A:416:LEU:HD22	2.04	0.40
1:B:196:SER:C	1:B:207:ASN:HD22	2.21	0.40
1:B:838:GLU:O	1:B:840:VAL:N	2.53	0.40
1:B:88:LEU:C	1:B:88:LEU:HD23	2.42	0.40
1:A:142:LEU:HD23	1:A:200:LEU:CD2	2.50	0.40
1:A:166:PHE:HD1	1:A:167:TYR:CD2	2.40	0.40
1:B:194:HIS:ND1	1:B:214:CYS:SG	2.93	0.40
1:B:251:LEU:HD13	1:B:418:ILE:HD12	2.02	0.40
1:B:18:TYR:HD1	1:B:26:PHE:CD1	2.39	0.40
1:B:969:ASP:O	1:B:972:LEU:CB	2.68	0.40
1:A:1074:PRO:C	1:A:1076:VAL:N	2.74	0.40
1:A:1316:VAL:HA	1:A:1319:GLU:CB	2.51	0.40
1:A:628:PRO:O	1:A:629:ARG:C	2.59	0.40
1:A:701:ARG:HA	1:A:730:LEU:HA	2.03	0.40
1:A:71:GLN:HB3	1:A:92:LEU:HD22	2.03	0.40
1:B:166:PHE:HD1	1:B:167:TYR:CD2	2.39	0.40
1:B:481:VAL:HB	1:B:490:SER:O	2.21	0.40
1:A:1207:ASN:O	1:A:1208:MET:C	2.59	0.40
1:A:1437:MET:C	1:A:1439:GLU:N	2.75	0.40
1:A:66:TYR:HD1	1:A:69:GLN:OE1	2.03	0.40
1:B:1028:LEU:O	1:B:1030:PHE:N	2.54	0.40
1:B:148:ARG:HG2	1:B:150:THR:HG22	2.03	0.40
1:B:29:THR:HG23	1:B:125:HIS:CD2	2.56	0.40
1:B:315:ALA:O	1:B:355:LEU:HA	2.22	0.40
1:B:840:VAL:O	1:B:841:GLU:C	2.59	0.40
1:B:88:LEU:O	1:B:92:LEU:HD12	2.21	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:O	1:A:1393:GLU:N[2_655]	1.65	0.55
1:A:116:GLN:NE2	1:A:1391:TYR:O[2_655]	1.85	0.35
1:A:117:TYR:H	1:A:1392:THR:O[2_655]	1.45	0.15
1:A:175:SER:H	1:A:1395:LYS:N[2_655]	1.51	0.09
1:A:174:ASP:O	1:A:1392:THR:C[2_655]	2.11	0.09
1:A:117:TYR:N	1:A:1392:THR:O[2_655]	2.14	0.06
1:A:116:GLN:HE21	1:A:1391:TYR:O[2_655]	1.55	0.05
1:A:109:LYS:N	1:A:1288:ASN:O[2_655]	2.18	0.02

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	1231/1581 (78%)	891 (72%)	234 (19%)	106 (9%)	1	15
1	B	1231/1581 (78%)	894 (73%)	228 (18%)	109 (9%)	1	15
All	All	2462/3162 (78%)	1785 (72%)	462 (19%)	215 (9%)	1	15

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	383	PRO
1	A	587	TYR
1	A	602	ASN
1	A	604	LYS
1	A	628	PRO
1	A	645	ILE
1	A	658	ASN
1	A	666	ILE
1	A	702	ASP

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Mol	Chain	Res	Type
1	A	708	ARG
1	A	744	CYS
1	A	762	ASP
1	A	789	HIS
1	A	863	THR
1	A	961	GLU
1	A	977	ILE
1	A	990	ILE
1	A	994	LEU
1	A	1133	VAL
1	A	1239	GLU
1	A	1243	ASN
1	A	1264	ASN
1	A	1286	GLU
1	A	1288	ASN
1	A	1299	ILE
1	A	1343	VAL
1	A	1347	ASP
1	A	1370	PRO
1	A	1394	ILE
1	A	1400	LEU
1	A	1418	VAL
1	A	1435	VAL
1	A	1437	MET
1	A	1458	CYS
1	A	1460	ALA
1	A	1461	CYS
1	B	48	ASN
1	B	200	LEU
1	B	286	VAL
1	B	383	PRO
1	B	587	TYR
1	B	625	ASN
1	B	628	PRO
1	B	640	SER
1	B	658	ASN
1	B	659	PRO
1	B	666	ILE
1	B	669	LYS
1	B	715	LEU
1	B	836	THR
1	B	838	GLU

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Mol	Chain	Res	Type
1	B	853	PRO
1	B	859	LYS
1	B	860	ASN
1	B	863	THR
1	B	898	VAL
1	B	961	GLU
1	B	990	ILE
1	B	1119	LEU
1	B	1201	GLN
1	B	1202	GLN
1	B	1221	PRO
1	B	1264	ASN
1	B	1267	ILE
1	B	1288	ASN
1	B	1299	ILE
1	B	1346	ASN
1	B	1370	PRO
1	B	1394	ILE
1	B	1400	LEU
1	B	1418	VAL
1	B	1458	CYS
1	B	1461	CYS
1	B	1464	THR
1	A	105	THR
1	A	226	TRP
1	A	550	ARG
1	A	640	SER
1	A	647	VAL
1	A	669	LYS
1	A	684	GLU
1	A	755	ILE
1	A	760	ASP
1	A	787	HIS
1	A	790	VAL
1	A	836	THR
1	A	853	PRO
1	A	895	LEU
1	A	1108	ASP
1	A	1109	VAL
1	A	1208	MET
1	A	1267	ILE
1	A	1301	THR

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Mol	Chain	Res	Type
1	A	1311	PHE
1	A	1349	ALA
1	A	1464	THR
1	B	226	TRP
1	B	396	ASN
1	B	550	ARG
1	B	638	CYS
1	B	670	LEU
1	B	708	ARG
1	B	839	PHE
1	B	861	LYS
1	B	864	PHE
1	B	888	THR
1	B	1028	LEU
1	B	1051	ASP
1	B	1053	ASP
1	B	1058	ARG
1	B	1109	VAL
1	B	1117	GLN
1	B	1208	MET
1	B	1216	GLU
1	B	1239	GLU
1	B	1292	VAL
1	B	1311	PHE
1	B	1347	ASP
1	B	1463	ASN
1	A	428	GLU
1	A	575	ALA
1	A	610	ILE
1	A	660	THR
1	A	682	THR
1	A	716	ALA
1	A	719	ALA
1	A	725	GLU
1	A	827	ASP
1	A	1028	LEU
1	A	1207	ASN
1	A	1414	CYS
1	A	1463	ASN
1	A	1474	LEU
1	B	50	PRO
1	B	291	PRO

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Mol	Chain	Res	Type
1	B	399	VAL
1	B	577	GLN
1	B	581	MET
1	B	589	VAL
1	B	591	ALA
1	B	604	LYS
1	B	693	GLU
1	B	714	GLU
1	B	726	ASP
1	B	727	ARG
1	B	787	HIS
1	B	789	HIS
1	B	790	VAL
1	B	827	ASP
1	B	837	MET
1	B	1133	VAL
1	B	1207	ASN
1	B	1301	THR
1	B	1322	PHE
1	B	1358	MET
1	B	1414	CYS
1	A	53	PHE
1	A	445	PHE
1	A	572	GLU
1	A	607	GLU
1	A	659	PRO
1	A	698	LEU
1	A	715	LEU
1	A	773	LEU
1	A	978	LEU
1	A	1004	SER
1	A	1075	LEU
1	A	1104	VAL
1	A	1355	ILE
1	A	1462	ASN
1	B	47	ASN
1	B	413	PRO
1	B	607	GLU
1	B	682	THR
1	B	720	LYS
1	B	858	GLU
1	B	981	ILE

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Mol	Chain	Res	Type
1	B	1081	GLN
1	B	1349	ALA
1	B	1356	GLN
1	B	1416	PRO
1	A	110	LEU
1	A	269	ARG
1	A	573	TYR
1	A	753	ASN
1	A	754	GLU
1	A	1074	PRO
1	A	1201	GLN
1	A	1202	GLN
1	A	1342	LEU
1	A	1397	ASN
1	A	1411	HIS
1	B	702	ASP
1	B	880	ASN
1	B	885	LEU
1	A	413	PRO
1	A	586	GLY
1	A	589	VAL
1	A	743	MET
1	B	593	ASP
1	B	645	ILE
1	B	684	GLU
1	B	745	LEU
1	B	773	LEU
1	B	852	PHE
1	B	854	PHE
1	A	286	VAL
1	B	647	VAL
1	B	1220	ILE
1	A	1221	PRO
1	B	497	VAL
1	A	646	PRO
1	B	498	VAL
1	A	984	VAL

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	400/1427 (28%)	356 (89%)	44 (11%)	7	30
1	B	400/1427 (28%)	360 (90%)	40 (10%)	9	33
All	All	800/2854 (28%)	716 (90%)	84 (10%)	8	32

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	28	SER
1	A	38	VAL
1	A	39	VAL
1	A	42	GLU
1	A	71	GLN
1	A	83	THR
1	A	101	LYS
1	A	102	GLN
1	A	105	THR
1	A	109	LYS
1	A	113	THR
1	A	117	TYR
1	A	121	ILE
1	A	127	LYS
1	A	142	LEU
1	A	150	THR
1	A	163	ILE
1	A	164	GLN
1	A	169	LEU
1	A	201	VAL
1	A	202	ASP
1	A	222	LEU
1	A	235	LYS
1	A	247	GLN
1	A	252	THR
1	A	255	GLU
1	A	289	HIS
1	A	302	LEU
1	A	317	GLU
1	A	356	VAL

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Mol	Chain	Res	Type
1	A	390	LEU
1	A	394	CYS
1	A	418	ILE
1	A	423	LEU
1	A	428	GLU
1	A	433	VAL
1	A	456	ILE
1	A	465	ILE
1	A	471	ARG
1	A	499	PHE
1	A	515	ILE
1	A	523	LEU
1	A	551	HIS
1	B	27	ILE
1	B	38	VAL
1	B	39	VAL
1	B	42	GLU
1	B	71	GLN
1	B	83	THR
1	B	97	ASP
1	B	101	LYS
1	B	105	THR
1	B	121	ILE
1	B	127	LYS
1	B	132	LEU
1	B	142	LEU
1	B	143	GLU
1	B	164	GLN
1	B	169	LEU
1	B	201	VAL
1	B	222	LEU
1	B	235	LYS
1	B	247	GLN
1	B	252	THR
1	B	255	GLU
1	B	258	LYS
1	B	302	LEU
1	B	317	GLU
1	B	356	VAL
1	B	390	LEU
1	B	394	CYS
1	B	397	THR

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Mol	Chain	Res	Type
1	B	411	GLU
1	B	418	ILE
1	B	428	GLU
1	B	433	VAL
1	B	436	SER
1	B	471	ARG
1	B	502	PRO
1	B	523	LEU
1	B	551	HIS
1	B	555	LEU
1	B	567	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	122	GLN
1	A	194	HIS
1	A	198	HIS
1	A	513	GLN
1	B	10	HIS
1	B	69	GLN
1	B	194	HIS
1	B	198	HIS
1	B	207	ASN
1	B	244	HIS

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	I3P	A	3000	-	24,24,24	1.10	3 (12%)	36,39,39	1.06	3 (8%)
2	I3P	B	3000	-	24,24,24	1.07	1 (4%)	36,39,39	1.07	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I3P	A	3000	-	-	0/15/39/39	0/1/1/1
2	I3P	B	3000	-	-	0/15/39/39	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	I3P	P5-O53	-2.07	1.46	1.54
2	A	3000	I3P	P4-O42	-2.06	1.46	1.54
2	A	3000	I3P	P1-O13	-2.03	1.46	1.54
2	B	3000	I3P	P1-O13	-2.01	1.46	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	I3P	O5-P5-O51	-2.34	100.10	109.26
2	B	3000	I3P	O1-C1-C2	2.09	113.53	108.66
2	A	3000	I3P	O1-C1-C2	2.10	113.55	108.66
2	B	3000	I3P	O53-P5-O52	2.19	116.45	107.61
2	B	3000	I3P	O43-P4-O42	2.26	116.74	107.61
2	A	3000	I3P	O13-P1-O12	2.40	117.31	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1491:SER	C	1492:SER	N	1.61

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	1257/1581 (79%)	0.48	163 (12%)	4 10	165, 174, 178, 180	0
1	B	1257/1581 (79%)	0.38	138 (10%)	6 12	165, 174, 178, 180	0
All	All	2514/3162 (79%)	0.43	301 (11%)	5 12	165, 174, 178, 180	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	THR	8.7
1	A	1389	ASN	8.4
1	B	253	CYS	8.0
1	B	279	LYS	8.0
1	B	388	VAL	7.6
1	A	58	PHE	7.4
1	A	265	ARG	7.3
1	B	184	LEU	7.0
1	A	1260	ASN	6.9
1	B	387	TYR	6.8
1	A	1391	TYR	6.7
1	A	1243	ASN	6.6
1	B	252	THR	6.3
1	B	280	ALA	6.3
1	A	118	GLY	6.2
1	A	211	SER	6.0
1	A	16	SER	5.9
1	A	1388	LYS	5.8
1	A	317	GLU	5.8
1	A	1414	CYS	5.7
1	A	119	ASN	5.7
1	A	318	VAL	5.7
1	A	1390	VAL	5.6
1	A	355	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	388	VAL	5.5
1	A	27	ILE	5.5
1	B	132	LEU	5.4
1	A	1240	PHE	5.3
1	B	282	TRP	5.3
1	B	27	ILE	5.3
1	B	56	CYS	5.2
1	A	390	LEU	5.2
1	A	60	LEU	5.1
1	A	1234	MET	5.1
1	B	307	HIS	5.1
1	B	1401	PRO	5.1
1	A	1244	PHE	5.0
1	A	59	LYS	5.0
1	A	1238	HIS	5.0
1	B	205	GLY	5.0
1	A	1242	GLN	4.9
1	A	215	ASN	4.9
1	B	123	LEU	4.9
1	B	390	LEU	4.8
1	A	1233	ILE	4.7
1	A	1392	THR	4.7
1	B	121	ILE	4.7
1	B	278	SER	4.7
1	A	132	LEU	4.7
1	B	119	ASN	4.6
1	A	1387	GLY	4.5
1	A	1239	GLU	4.5
1	A	131	TYR	4.5
1	B	1402	LEU	4.4
1	B	185	ASN	4.4
1	B	162	TYR	4.4
1	B	52	LYS	4.4
1	A	28	SER	4.4
1	A	1413	ASP	4.4
1	B	825	SER	4.4
1	A	64	ASN	4.4
1	A	234	LEU	4.4
1	A	554	ARG	4.4
1	A	56	CYS	4.4
1	B	122	GLN	4.4
1	B	309	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1134	TYR	4.3
1	B	53	PHE	4.3
1	B	250	PHE	4.3
1	A	17	LEU	4.3
1	B	1403	ASP	4.2
1	A	205	GLY	4.2
1	B	372	PRO	4.2
1	A	1450	PHE	4.2
1	B	310	THR	4.1
1	B	1189	GLN	4.1
1	A	399	VAL	4.1
1	A	182	VAL	4.1
1	A	6	SER	4.1
1	A	63	MET	4.1
1	B	251	LEU	4.0
1	A	556	CYS	4.0
1	A	253	CYS	4.0
1	A	116	GLN	4.0
1	A	123	LEU	3.9
1	B	277	SER	3.9
1	B	370	LEU	3.9
1	A	153	GLU	3.9
1	A	279	LYS	3.9
1	B	305	PHE	3.9
1	A	267	THR	3.9
1	A	354	SER	3.9
1	A	414	VAL	3.9
1	A	254	ASP	3.9
1	B	1404	ASP	3.9
1	B	265	ARG	3.8
1	B	553	CYS	3.8
1	A	557	TYR	3.8
1	B	1279	ASN	3.8
1	A	166	PHE	3.7
1	A	1221	PRO	3.7
1	B	1190	GLU	3.7
1	B	161	PHE	3.7
1	B	183	VAL	3.7
1	A	419	GLY	3.7
1	A	188	ASN	3.7
1	A	1451	GLU	3.6
1	B	62	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1241	LEU	3.6
1	A	249	LYS	3.6
1	A	1310	LYS	3.6
1	A	1222	TYR	3.6
1	B	193	LEU	3.6
1	B	153	GLU	3.6
1	A	1046	GLU	3.5
1	A	1237	ALA	3.5
1	B	382	VAL	3.5
1	A	1184	SER	3.5
1	B	1397	ASN	3.5
1	A	183	VAL	3.5
1	B	1478	VAL	3.5
1	A	1368	ASN	3.5
1	B	54	ARG	3.4
1	A	370	LEU	3.4
1	B	1400	LEU	3.4
1	B	234	LEU	3.4
1	A	667	GLU	3.4
1	B	826	LYS	3.4
1	A	560	LEU	3.4
1	B	1247	GLY	3.4
1	A	1488	THR	3.4
1	A	1232	GLU	3.4
1	B	1187	CYS	3.3
1	A	389	ARG	3.3
1	B	22	SER	3.3
1	A	152	ASP	3.3
1	B	283	GLU	3.3
1	A	252	THR	3.3
1	A	1230	MET	3.3
1	A	124	LEU	3.2
1	B	1481	ILE	3.2
1	A	356	VAL	3.2
1	B	649	GLN	3.2
1	A	553	CYS	3.2
1	B	163	ILE	3.2
1	A	1259	ILE	3.1
1	B	281	LEU	3.1
1	B	1185	LYS	3.1
1	B	1244	PHE	3.1
1	A	15	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	120	VAL	3.1
1	B	1188	VAL	3.1
1	B	299	TRP	3.1
1	A	191	GLN	3.1
1	B	1191	SER	3.1
1	B	430	PHE	3.1
1	A	62	PRO	3.1
1	B	1238	HIS	3.1
1	B	1246	ALA	3.0
1	B	1479	THR	3.0
1	A	561	ARG	3.0
1	B	429	ALA	3.0
1	B	61	CYS	3.0
1	B	564	GLN	3.0
1	A	1133	VAL	3.0
1	A	1223	GLU	3.0
1	B	402	THR	2.9
1	B	1480	GLU	2.9
1	B	1389	ASN	2.9
1	A	151	LEU	2.9
1	A	382	VAL	2.9
1	A	668	THR	2.9
1	A	1412	GLU	2.9
1	B	266	THR	2.8
1	A	559	VAL	2.8
1	B	1282	GLN	2.8
1	A	1229	LYS	2.8
1	A	55	ASP	2.8
1	A	164	GLN	2.8
1	B	1108	ASP	2.8
1	A	1491	SER	2.8
1	A	284	VAL	2.8
1	B	351	MET	2.8
1	A	1235	ARG	2.8
1	B	1482	VAL	2.7
1	B	1237	ALA	2.7
1	B	9	LEU	2.7
1	B	118	GLY	2.7
1	A	216	THR	2.7
1	B	587	TYR	2.7
1	A	115	ILE	2.7
1	B	40	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	195	ALA	2.6
1	B	386	SER	2.6
1	B	422	PRO	2.6
1	A	1246	ALA	2.6
1	A	1415	ILE	2.6
1	A	1369	SER	2.6
1	A	57	LEU	2.6
1	A	309	ALA	2.6
1	B	738	ASN	2.6
1	A	1266	GLY	2.6
1	A	117	TYR	2.6
1	B	131	TYR	2.6
1	A	193	LEU	2.5
1	A	250	PHE	2.5
1	A	1386	GLU	2.5
1	A	22	SER	2.5
1	A	1180	LEU	2.5
1	A	210	ASN	2.5
1	B	1059	THR	2.5
1	B	60	LEU	2.5
1	A	563	SER	2.5
1	B	663	ASP	2.5
1	A	1433	THR	2.5
1	B	152	ASP	2.5
1	A	1343	VAL	2.5
1	B	1243	ASN	2.5
1	A	122	GLN	2.5
1	A	1269	GLU	2.5
1	A	163	ILE	2.4
1	A	220	ILE	2.4
1	B	1370	PRO	2.4
1	A	154	ALA	2.4
1	B	1433	THR	2.4
1	B	59	LYS	2.4
1	A	1339	GLU	2.4
1	B	241	ARG	2.4
1	B	371	ASP	2.4
1	A	189	ALA	2.4
1	A	383	PRO	2.4
1	A	315	ALA	2.4
1	A	52	LYS	2.4
1	A	1045	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	39	VAL	2.4
1	A	666	ILE	2.4
1	A	1490	PHE	2.3
1	A	1487	THR	2.3
1	B	1278	MET	2.3
1	B	1066	HIS	2.3
1	B	209	VAL	2.3
1	B	254	ASP	2.3
1	B	648	THR	2.3
1	B	976	GLU	2.3
1	B	28	SER	2.3
1	A	1340	ASP	2.3
1	B	1045	GLU	2.3
1	A	1261	LEU	2.3
1	A	558	ARG	2.3
1	A	214	CYS	2.3
1	A	149	VAL	2.3
1	B	17	LEU	2.2
1	B	1484	SER	2.2
1	A	430	PHE	2.2
1	B	1046	GLU	2.2
1	A	413	PRO	2.2
1	A	386	SER	2.2
1	B	1274	GLN	2.2
1	A	61	CYS	2.2
1	B	497	VAL	2.2
1	A	106	GLU	2.2
1	B	218	TRP	2.2
1	A	130	LYS	2.2
1	B	731	SER	2.2
1	B	1388	LYS	2.2
1	A	774	PRO	2.2
1	A	9	LEU	2.2
1	A	314	LEU	2.2
1	B	1398	SER	2.2
1	B	311	GLY	2.1
1	B	1485	ILE	2.1
1	A	1110	ASP	2.1
1	B	314	LEU	2.1
1	B	306	LYS	2.1
1	B	549	PHE	2.1
1	A	150	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	300	ASN	2.1
1	A	1228	THR	2.1
1	B	243	PHE	2.1
1	A	1231	GLN	2.1
1	B	827	ASP	2.1
1	A	1270	ALA	2.1
1	B	1432	ASP	2.1
1	B	164	GLN	2.1
1	A	65	ARG	2.1
1	B	1280	ASN	2.1
1	A	176	VAL	2.1
1	A	133	THR	2.1
1	B	389	ARG	2.1
1	B	308	LEU	2.0
1	B	1184	SER	2.0
1	B	273	THR	2.0
1	B	560	LEU	2.0
1	B	1277	PHE	2.0
1	A	1484	SER	2.0
1	A	742	ARG	2.0
1	B	417	LYS	2.0
1	A	1452	ASN	2.0
1	A	37	CYS	2.0
1	A	1185	LYS	2.0
1	A	1385	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	I3P	B	3000	24/24	0.87	0.45	-0.21	174,174,174,174	0
2	I3P	A	3000	24/24	0.72	0.65	-0.22	174,174,174,174	0

6.5 Other polymers [i](#)

There are no such residues in this entry.