



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:10 PM UTC

PDB ID : 5GUG / pdb_00005gug
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain with inositol 1,4,5-trisphosphate
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2016-08-29
Resolution : 7.40 Å(reported)

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

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

A user guide is available at

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

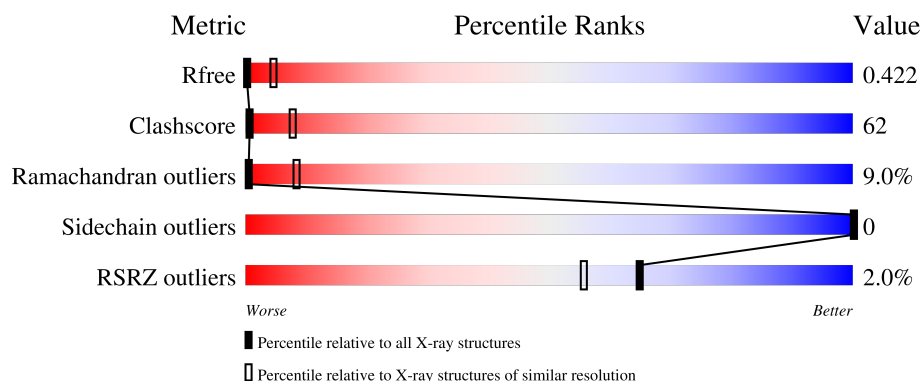
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 ≥ 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	2217	% 40% 32% 5% 22%
1	B	2217	2% 40% 32% 6% 22%

2 Entry composition [i](#)

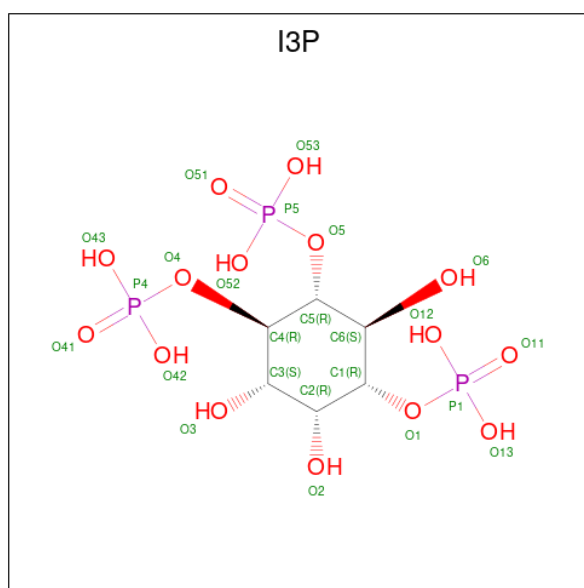
There are 2 unique types of molecules in this entry. The entry contains 25117 atoms, of which 7810 are hydrogens and 0 are deuteriums.

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	1721	Total	C	H	N	O	S	0	0	0
			12529	5147	3897	1746	1738	1			
1	B	1720	Total	C	H	N	O	S	0	0	0
			12522	5144	3895	1745	1737	1			

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

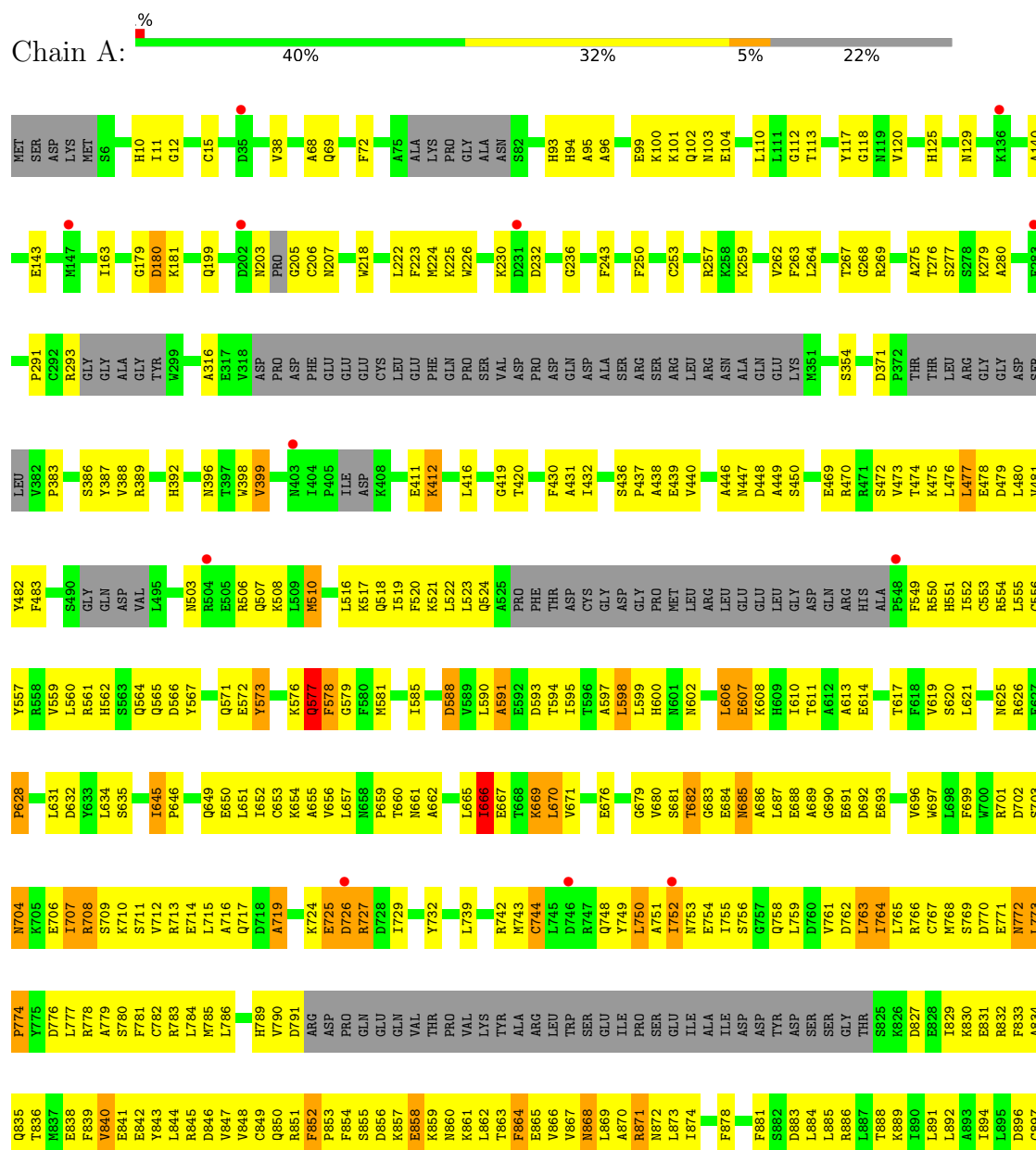


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			33	6	9	15	3		
2	B	1	Total	C	H	O	P	0	0
			33	6	9	15	3		

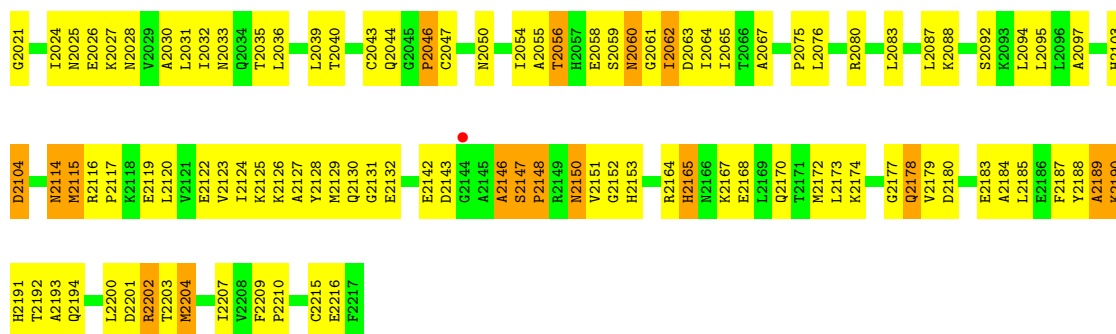
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

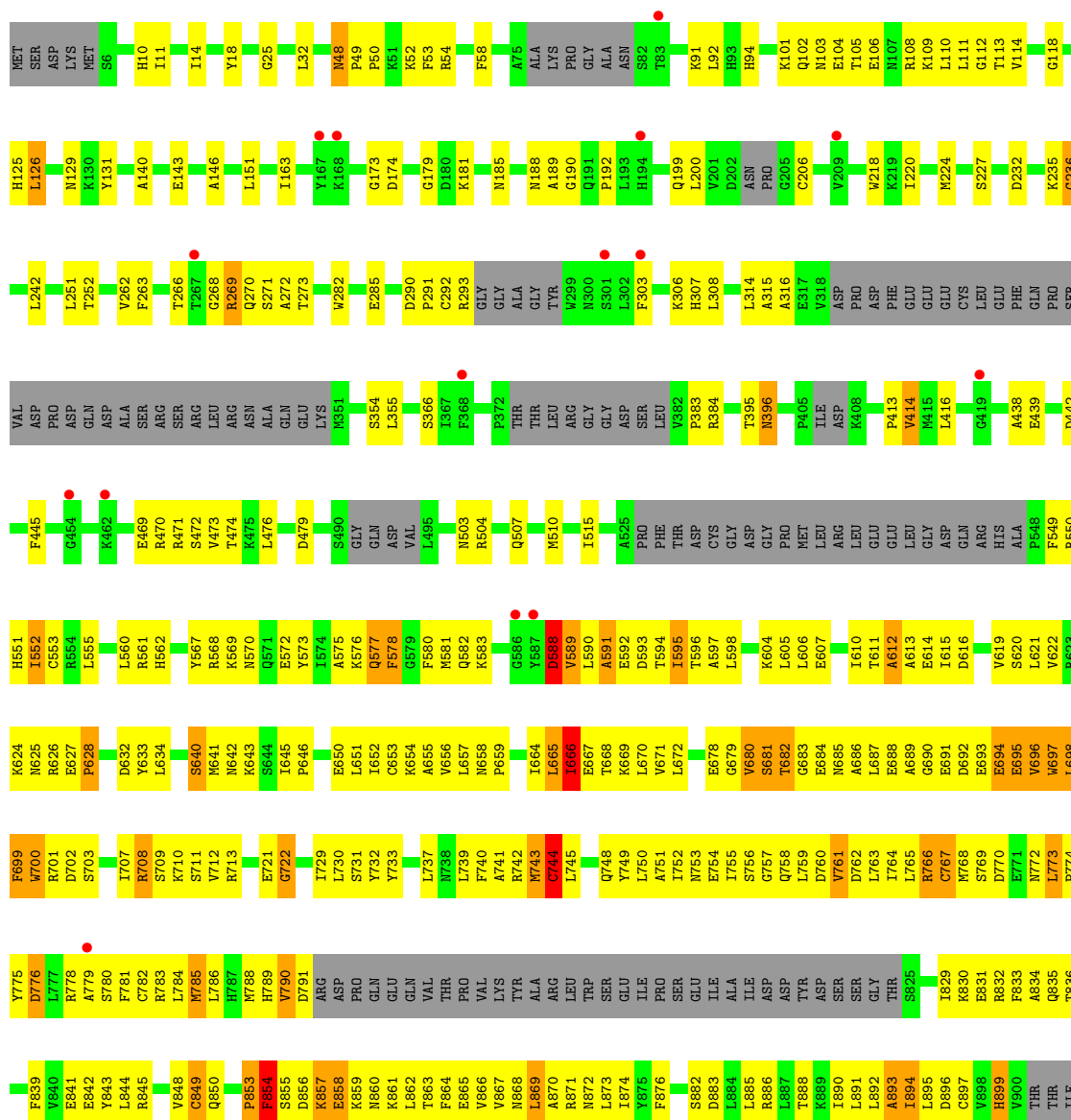
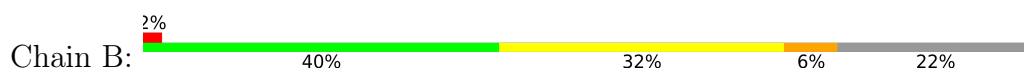
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



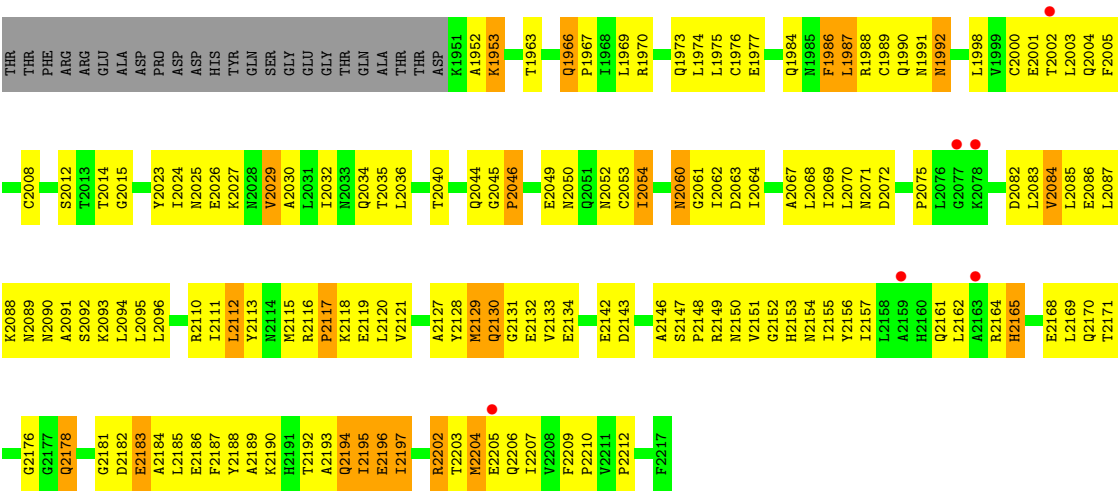




● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



PHE	1965	F1041	K1116	I1179	Q1250	D1347	L1449	MET	ARG	L1662	GLU	GLY	F1856
PRO	M966	G1042	Q1117	R1182	N1261	D1350	F1453	PRO	ARG	L1663	ASP	GLU	K1857
ILE	V967	G1043	D1118	L1183	Q1262	F1351	F1453	SER	ASP	E1664	HIS	GLY	V1858
SER	M968	E1046	L1119	L1190	K1257	L1354	D1456	GLN	SER	E1665	LYS	ARG	F1859
LYS	D969	D1051	L1122	E1190	H1258	L1355	R1459	LYS	VAL	E1667	GLY	GLY	Y1860
MET	T970	L1052	V1126	S1191	H1269	Q1356	A1460	ALA	ALA	E1668	GLU	ALA	M1863
THR	K971	D1053	E1127	A1192	E1269	Q1356	A1460	SER	ALA	C1671	LEU	ALA	K1864
LYS	L972	H1054	K1128	A1192	E1270	D1363	R1462	VAL	ALA	T1677	LEU	ALA	L1867
GLY	K973	H1055	S1129	V1194	V1271	D1363	R1462	GLY	ALA	T1677	GLN	ARG	Q1867
GLU	I974	H1055	E1130	S1197	T1272	P1370	A1470	CYS	ALA	L1678	ILE	ILE	L1871
ASN	E976	G1056	E1131	R1198	H1275	H1376	A1470	ILE	ARG	R1679	ARG	LEU	K1872
LYS	I977	R1058	W1132	K1199	L1276	V1377	D1471	VAL	VAL	E1680	VAL	VAL	L1872
GLY	L978	T1059	V1133	Q1201	L1277	V1378	K1476	LEU	LEU	M1681	ASN	ASN	T1873
SER	Q979	F1060	Y1134	Q1201	M1278	E1379	K1476	LEU	SER	M1682	ARG	ARG	V1874
ASN	F880	L1061	LYS	Q1202	N1279	E1380	E1480	ASP	ASP	T1683	TYR	TYR	E1801
VAL	I981	R1062	GLY	R1203	M1280	L1381	E1480	VAL	ALA	K1684	GLY	GLY	G1802
MET	L982	V1063	GLN	Q1203	F1281	L1382	M1483	VAL	LYS	D1685	GLY	ASN	M1805
ARG	N983	L1064	GLY	G1209	Q1282	V1383	S1484	ALA	SER	R1686	ILE	ILE	L1810
SER	V984	T1068	PRO	A1210	L1282	E1386	I1485	LYS	SER	T1687	ILE	ARG	N1813
ILE	R985	D1071	ASP	H1211	C1284	G1387	I1485	ALA	ARG	GLY	PRO	PRO	A1814
HIS	L986	Y1072	GLU	A1212	S1285	E1388	T1487	ALA	ALA	GLY	ARG	GLY	S1815
GLY	D987	F1073	PRO	V1213	E1286	K1388	T1487	ILE	ILE	LYS	GLY	GLY	S1816
VAL	Y988	P1074	MET	V1213	I1287	N1389	F1488	ILE	ILE	GLN	ARG	ARG	D1817
GLY	R989	P1074	ASP	L1215	N1288	M1397	S1492	ILE	PRO	ILE	ARG	ARG	R1818
GLU	I990	P1074	GLY	E1216	N1288	N1397	P1493	PRO	VAL	ILE	GLU	GLU	H1821
LEU	S991	L1075	ALA	L1217	R1290	L1400	P1493	VAL	ASP	GLY	GLY	GLY	I1822
MET	C992	L993	SER	L1218	R1291	L1400	P1493	ASP	LEU	GLY	GLY	GLY	S1823
THR	L994	L994	GLY	Q1219	V1292	L1400	P1493	ASP	ASP	GLY	GLY	GLY	I1824
GLN	VAL	A1079	GLU	I1220	Q1293	D1403	P1493	ASP	SER	GLY	GLY	GLY	L1825
VAL	F997	L1080	ASN	F1221	H1294	D1404	P1493	SER	SER	GLY	GLY	GLY	L1826
LEU	K998	Q1081	GLU	Y1222	E1294	D1404	P1493	GLN	GLN	GLY	GLY	GLY	A1827
ARG	R999	L1082	HIS	E1223	F1295	V1405	P1493	VAL	ASN	ALA	ASN	ASN	L1828
GLY	D1002	L1083	LYS	K1224	F1295	V1406	P1493	THR	THR	ALA	GLY	GLY	I1829
GLY	S1008	F1084	LYS	A1225	E1300	E1417	P1493	LEU	LEU	GLY	LEU	PRO	A1829
GLY	S1009	R1085	THR	E1226	T1301	V1418	P1493	LEU	LEU	GLY	PRO	PRO	GLY
PHE	S1008	H1086	GLU	D1227	T1301	V1418	P1493	PHE	PHE	GLY	LEU	LEU	THR
LEU	S1009	S1087	GLU	T1228	R1304	A1421	P1493	LEU	LEU	GLY	SER	SER	THR
PRO	THR	S1088	GLY	K1229	K1310	Y1422	P1493	LEU	LEU	GLY	PRO	PRO	GLN
MET	THR	V1093	THR	Q1231	F1311	Y1422	P1493	LYS	LYS	GLY	GLY	GLY	ILE
THR	SER	L1094	LYS	Q1231	L1312	L1426	P1493	HIS	ASN	GLY	PRO	PRO	GLY
PRO	SER	Q1095	PRO	E1233	Q1313	L1426	P1493	ASN	ASN	GLY	ALA	ALA	GLY
MET	GLY	A1096	LEU	M1234	T1314	P1431	P1493	ILE	ILE	ASN	VAL	VAL	LYS
ALA	ASN	F1097	LYS	R1235	I1315	D1432	P1493	VAL	VAL	ASN	GLN	GLN	PRO
ALA	SER	Q1098	HIS	L1236	V1316	T1433	P1493	GLN	GLN	GLY	LYS	LYS	PRO
PRO	GLN	Q1099	GLU	A1237	K1317	E1434	P1493	THR	THR	GLY	GLY	GLY	GLY
GLY	GLY	V1100	SER	H1238	A1318	V1435	P1493	ALA	ALA	GLY	GLY	GLY	GLY
GLY	GLY	Q1101	THR	E1239	C1326	E1436	P1493	LEU	LEU	GLY	GLY	GLY	GLY
ASN	PRO	L1102	SER	F1240	Q1327	M1437	P1493	ASN	ASN	LEU	GLY	GLY	GLY
VAL	SER	L1103	SER	L1241	D1328	K1438	P1493	TRP	TRP	GLY	GLY	GLY	GLY
LYS	ASN	V1104	TYR	Q1242	M1329	E1439	P1493	ARG	ARG	PRO	PRO	PRO	PRO
GLN	VAL	T1105	ASN	N1243	V1330	T1442	P1493	LEU	LEU	SER	SER	SER	SER
ALA	PRO	S1106	TYR	F1244	V1330	T1442	P1493	ALA	ALA	ALA	ALA	ALA	ALA
GLY	G1026	Q1107	ARG	C1245	V1341	H1444	P1493	ARG	ARG	LEU	LEU	LEU	LEU
P960	D1029	K1113	VAL	A1246	Y1345	H1444	P1493	ASN	ASN	GLY	GLY	GLY	GLY
K962	I1040	Q1114	K1177	G1247	Y1345	H1444	P1493	ALA	ALA	GLY	GLY	GLY	GLY
		I1115	E1178	Q1249	N1346	H1446	P1493	ALA	ALA	LEU	LEU	LEU	LEU



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.99Å 223.49Å 319.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 7.40 49.49 – 7.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.49-7.40) 85.7 (49.49-7.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.356 , 0.416 0.361 , 0.422	Depositor DCC
R_{free} test set	526 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	159.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 700.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.23$, $\langle L^2 \rangle = 0.08$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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	1.01	13/8617 (0.2%)	1.11	25/11978 (0.2%)
1	B	0.99	11/8612 (0.1%)	1.08	21/11971 (0.2%)
All	All	1.00	24/17229 (0.1%)	1.09	46/23949 (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	8
1	B	0	9
All	All	0	17

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	GLN	CA-C	11.22	1.68	1.52
1	B	270	GLN	CD-NE2	-11.09	1.09	1.33
1	A	577	GLN	C-O	10.33	1.37	1.24
1	B	270	GLN	CD-OE1	-8.94	1.06	1.23
1	B	588	ASP	C-O	7.90	1.32	1.23
1	B	666	ILE	CA-CB	-7.81	1.43	1.54
1	A	579	GLY	N-CA	-7.04	1.36	1.45
1	B	588	ASP	N-CA	-6.96	1.38	1.46
1	A	717	GLN	CA-CB	-6.82	1.41	1.53
1	A	1118	ASP	CA-CB	6.72	1.66	1.53
1	A	666	ILE	CA-C	6.60	1.61	1.52
1	A	772	ASN	CA-CB	6.23	1.64	1.53
1	A	772	ASN	C-N	6.15	1.46	1.33
1	B	1445	HIS	C-O	-5.76	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	GLN	CA-CB	-5.71	1.42	1.53
1	B	553	CYS	N-CA	-5.68	1.38	1.45
1	B	578	PHE	C-O	-5.63	1.16	1.24
1	B	589	VAL	CA-C	5.60	1.59	1.52
1	A	666	ILE	CA-CB	-5.41	1.47	1.54
1	B	1026	GLY	C-O	-5.41	1.12	1.23
1	B	578	PHE	CA-C	-5.30	1.45	1.52
1	A	120	VAL	C-N	5.15	1.43	1.33
1	A	1800	LYS	CA-CB	-5.11	1.45	1.52
1	A	578	PHE	C-N	-5.00	1.26	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	GLN	CA-C-N	12.85	144.83	121.70
1	A	577	GLN	C-N-CA	12.85	144.83	121.70
1	B	588	ASP	N-CA-C	10.31	129.24	107.70
1	A	578	PHE	N-CA-CB	8.83	125.51	110.50
1	B	553	CYS	N-CA-C	-8.20	99.48	110.55
1	B	2115	MET	N-CA-C	-7.50	97.92	109.24
1	B	588	ASP	N-CA-CB	-7.39	98.82	110.87
1	A	772	ASN	N-CA-C	-7.06	95.76	110.80
1	B	666	ILE	N-CA-C	6.56	122.98	109.34
1	A	666	ILE	N-CA-C	6.28	122.41	109.34
1	B	1270	ALA	N-CA-C	6.13	119.22	109.65
1	A	579	GLY	N-CA-C	-6.07	105.29	113.24
1	A	510	MET	CB-CG-SD	-6.01	94.68	112.70
1	A	772	ASN	CB-CA-C	5.90	122.16	110.42
1	A	1462	ASN	N-CA-C	-5.88	104.98	113.21
1	A	670	LEU	N-CA-C	5.74	119.81	112.34
1	B	1462	ASN	CA-C-N	5.68	132.40	121.54
1	B	1462	ASN	C-N-CA	5.68	132.40	121.54
1	B	1594	ARG	CA-C-N	5.68	131.43	122.11
1	B	1594	ARG	C-N-CA	5.68	131.43	122.11
1	B	1476	LYS	N-CA-CB	-5.59	100.67	109.78
1	B	743	MET	CA-C-O	-5.56	115.65	121.99
1	A	1220	ILE	N-CA-C	-5.54	105.75	112.67
1	A	999	ARG	N-CA-C	-5.46	100.77	109.07
1	A	868	ASN	N-CA-C	-5.41	102.49	111.37
1	A	774	PRO	N-CA-C	-5.41	101.33	112.47
1	B	355	LEU	N-CA-C	5.33	117.41	108.73
1	A	576	LYS	CA-C-N	5.32	130.88	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	LYS	C-N-CA	5.32	130.88	120.99
1	A	1420	ILE	CA-C-N	5.27	130.64	122.26
1	A	1420	ILE	C-N-CA	5.27	130.64	122.26
1	B	227	SER	N-CA-C	-5.26	102.30	109.71
1	B	1884	LYS	N-CA-C	5.24	125.67	111.00
1	A	591	ALA	CA-C-N	5.20	127.56	120.54
1	A	591	ALA	C-N-CA	5.20	127.56	120.54
1	A	72	PHE	CA-C-N	5.18	132.66	122.61
1	A	72	PHE	C-N-CA	5.18	132.66	122.61
1	B	414	VAL	N-CA-C	5.14	120.03	109.34
1	A	2115	MET	N-CA-C	-5.12	99.89	110.80
1	B	743	MET	CA-C-N	5.06	130.81	121.70
1	B	743	MET	C-N-CA	5.06	130.81	121.70
1	B	977	ILE	CA-C-N	5.04	131.16	121.54
1	B	977	ILE	C-N-CA	5.04	131.16	121.54
1	A	1461	CYS	N-CA-C	-5.03	100.09	110.80
1	B	854	PHE	N-CA-C	5.02	121.49	110.80
1	A	998	LYS	N-CA-C	-5.01	100.12	110.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	GLU	Peptide
1	A	1375	ILE	Peptide
1	A	1380	LEU	Peptide
1	A	1461	CYS	Peptide
1	A	2114	ASN	Peptide
1	A	2142	GLU	Peptide
1	A	577	GLN	Peptide
1	A	588	ASP	Peptide
1	B	1269	GLU	Peptide
1	B	1421	ALA	Peptide
1	B	1593	SER	Mainchain
1	B	1594	ARG	Peptide
1	B	1798	LEU	Peptide
1	B	577	GLN	Peptide
1	B	588	ASP	Peptide
1	B	744	CYS	Peptide
1	B	759	LEU	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	8632	3897	3899	762	0
1	B	8627	3895	3898	792	0
2	A	24	9	9	6	0
2	B	24	9	9	1	0
All	All	17307	7810	7815	1553	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 62.

All (1553) 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:2020:LEU:O	1:A:2024:ILE:N	1.57	1.38
1:B:863:THR:O	1:B:867:VAL:N	1.72	1.21
1:A:1210:ALA:O	1:A:1214:VAL:CB	1.89	1.20
1:A:1125:ILE:O	1:A:1129:SER:CB	1.91	1.19
1:B:1682:MET:O	1:B:1686:ARG:N	1.78	1.16
1:A:869:LEU:O	1:A:873:LEU:N	1.81	1.14
1:A:1864:LYS:O	1:A:1867:GLN:N	1.82	1.13
1:A:2124:ILE:O	1:A:2128:TYR:CB	2.00	1.09
1:A:866:VAL:O	1:A:870:ALA:N	1.87	1.08
1:A:2150:ASN:O	1:A:2153:HIS:N	1.87	1.08
1:B:1966:GLN:O	1:B:1970:ARG:CB	2.05	1.04
1:A:1421:ALA:O	1:A:1425:PHE:CB	2.04	1.04
1:A:1377:LEU:O	1:A:1381:LEU:CB	2.06	1.03
1:A:1231:GLN:O	1:A:1235:ARG:CB	2.05	1.03
1:A:1420:ILE:O	1:A:1424:ASN:CB	2.07	1.03
1:A:2125:LYS:O	1:A:2129:MET:CB	2.06	1.02
1:B:1635:LEU:O	1:B:1639:ASN:N	1.93	1.02
1:B:2061:GLY:O	1:B:2064:ILE:N	1.92	1.01
1:A:2147:SER:O	1:A:2151:VAL:CB	2.08	1.01
1:A:1371:LEU:O	1:A:1375:ILE:N	1.92	1.01
1:B:1231:GLN:O	1:B:1235:ARG:CB	2.09	1.00
1:A:1126:VAL:O	1:A:1130:GLU:CB	2.10	1.00
1:A:628:PRO:O	1:A:632:ASP:N	1.95	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:764:ILE:O	1:B:768:MET:N	1.96	0.98
1:A:1843:PHE:O	1:A:1846:LEU:N	1.93	0.98
1:A:1849:ASP:O	1:A:1853:GLU:N	1.96	0.98
1:B:2147:SER:O	1:B:2151:VAL:N	1.96	0.98
1:A:1252:GLN:O	1:A:1256:HIS:N	1.97	0.98
1:B:2091:ALA:O	1:B:2095:LEU:CB	2.12	0.97
1:B:2182:ASP:O	1:B:2185:LEU:N	1.97	0.97
1:B:763:LEU:O	1:B:767:CYS:N	1.97	0.97
1:A:844:LEU:O	1:A:847:VAL:N	1.98	0.96
1:A:476:LEU:O	1:A:479:ASP:N	1.98	0.96
1:A:978:LEU:O	1:A:982:LEU:N	1.98	0.95
1:B:785:MET:O	1:B:788:MET:N	1.99	0.95
1:A:976:GLU:O	1:A:980:PHE:N	2.00	0.94
1:A:868:ASN:O	1:A:872:ASN:N	1.99	0.94
1:B:782:CYS:O	1:B:785:MET:N	2.01	0.93
1:A:1867:GLN:O	1:A:1871:LYS:CB	2.16	0.93
1:B:620:SER:O	1:B:624:LYS:N	2.02	0.93
1:A:708:ARG:O	1:A:712:VAL:N	2.02	0.92
1:A:1179:ILE:O	1:A:1183:LEU:CB	2.17	0.92
1:B:780:SER:O	1:B:783:ARG:N	2.02	0.92
1:A:552:ILE:O	1:A:556:CYS:N	2.02	0.92
1:B:1417:GLU:O	1:B:1421:ALA:N	2.03	0.91
1:A:1472:SER:O	1:A:1476:LYS:CB	2.19	0.91
1:A:1820:PHE:O	1:A:1824:ILE:N	2.03	0.91
1:A:2188:TYR:O	1:A:2192:THR:CB	2.19	0.91
1:A:651:LEU:O	1:A:655:ALA:N	2.04	0.91
1:B:1096:ALA:O	1:B:1100:VAL:N	2.03	0.91
1:A:867:VAL:O	1:A:871:ARG:N	2.03	0.90
1:A:354:SER:HA	1:A:419:GLY:HA2	1.54	0.90
1:B:891:LEU:O	1:B:895:LEU:CB	2.19	0.90
1:B:1422:TYR:O	1:B:1426:LEU:CB	2.19	0.90
1:B:2050:ASN:O	1:B:2054:ILE:CB	2.19	0.90
1:B:476:LEU:O	1:B:479:ASP:N	2.05	0.90
1:A:1118:ASP:O	1:A:1121:GLN:N	2.05	0.89
1:A:650:GLU:O	1:A:654:LYS:N	2.06	0.89
1:B:621:LEU:O	1:B:625:ASN:N	2.07	0.88
1:A:2055:ALA:O	1:A:2059:SER:N	2.06	0.88
1:A:2021:GLY:O	1:A:2025:ASN:N	2.07	0.88
1:A:2128:TYR:O	1:A:2132:GLU:CB	2.22	0.88
1:A:125:HIS:O	1:A:129:ASN:N	2.07	0.88
1:B:665:LEU:O	1:B:671:VAL:N	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1986:PHE:O	1:B:1988:ARG:N	2.07	0.87
1:B:789:HIS:O	1:B:791:ASP:N	2.06	0.87
1:A:833:PHE:O	1:A:836:THR:N	2.07	0.87
1:A:1294:HIS:O	1:A:1298:CYS:N	2.06	0.87
1:B:866:VAL:O	1:B:870:ALA:N	2.07	0.87
1:B:1119:LEU:O	1:B:1122:LEU:N	2.07	0.87
1:A:1817:ASP:O	1:A:1821:HIS:N	2.05	0.87
1:B:1821:HIS:O	1:B:1825:LEU:N	2.08	0.87
1:B:1849:ASP:O	1:B:1852:SER:N	2.08	0.87
1:A:1862:ARG:O	1:A:1866:ALA:CB	2.23	0.86
1:A:585:ILE:HA	1:A:591:ALA:HB1	1.57	0.86
1:A:1417:GLU:O	1:A:1419:LYS:N	2.08	0.86
1:A:2126:LYS:O	1:A:2130:GLN:CB	2.24	0.86
1:B:2183:GLU:O	1:B:2187:PHE:CB	2.23	0.86
1:A:268:GLY:N	2:A:3000:I3P:O42	2.08	0.85
1:B:1797:HIS:O	1:B:1802:GLY:N	2.09	0.85
1:A:1116:LYS:O	1:A:1119:LEU:N	2.08	0.85
1:A:2076:LEU:HA	1:A:2080:ARG:CB	2.07	0.85
1:B:872:ASN:O	1:B:876:PHE:N	2.08	0.85
1:A:267:THR:OG1	2:A:3000:I3P:O41	1.94	0.85
1:A:710:LYS:O	1:A:714:GLU:N	2.10	0.84
1:B:1223:GLU:O	1:B:1271:VAL:CB	2.25	0.84
1:A:269:ARG:NH2	2:A:3000:I3P:O52	2.09	0.84
1:A:2004:GLN:O	1:A:2008:CYS:N	2.11	0.84
1:B:967:VAL:O	1:B:969:ASP:N	2.10	0.84
1:B:2148:PRO:O	1:B:2152:GLY:N	2.11	0.84
1:A:975:ILE:O	1:A:979:GLN:N	2.09	0.84
1:B:1211:HIS:O	1:B:1214:VAL:N	2.10	0.83
1:B:885:LEU:O	1:B:888:THR:N	2.09	0.83
1:B:1986:PHE:O	1:B:1989:CYS:N	2.12	0.83
1:A:1379:GLU:HA	1:A:1382:ALA:HB3	1.59	0.83
1:B:2128:TYR:O	1:B:2132:GLU:CB	2.26	0.83
1:B:552:ILE:O	1:B:555:LEU:N	2.11	0.83
1:A:1208:MET:O	1:A:1212:ALA:CB	2.26	0.83
1:A:773:LEU:CB	1:A:779:ALA:H	1.92	0.83
1:A:1792:ALA:O	1:A:1796:CYS:CB	2.27	0.82
1:A:773:LEU:CB	1:A:779:ALA:N	2.43	0.82
1:B:11:ILE:O	1:B:112:GLY:N	2.11	0.82
1:B:680:VAL:O	1:B:682:THR:N	2.12	0.82
1:B:773:LEU:O	1:B:775:TYR:N	2.12	0.82
1:B:988:TYR:O	1:B:990:ILE:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:GLN:O	1:A:573:TYR:N	2.13	0.81
1:A:1317:LYS:HA	1:A:1323:ILE:CB	2.09	0.81
1:A:665:LEU:O	1:A:671:VAL:N	2.14	0.81
1:A:1862:ARG:O	1:A:1866:ALA:HB3	1.78	0.81
1:B:864:PHE:O	1:B:868:ASN:N	2.13	0.81
1:B:2152:GLY:O	1:B:2156:TYR:CB	2.30	0.80
1:A:1118:ASP:O	1:A:1120:ASP:N	2.13	0.80
1:A:708:ARG:O	1:A:712:VAL:CB	2.29	0.80
1:A:982:LEU:O	1:A:986:LEU:N	2.14	0.79
1:B:1095:GLN:O	1:B:1099:GLN:N	2.13	0.79
1:B:1609:ALA:O	1:B:1613:ARG:CB	2.31	0.79
1:B:1638:GLU:O	1:B:1640:THR:N	2.15	0.79
1:A:1992:ASN:O	1:A:1994:THR:N	2.15	0.78
1:A:2007:ASP:O	1:A:2011:GLY:N	2.16	0.78
1:A:2036:LEU:O	1:A:2040:THR:CB	2.30	0.78
1:A:970:THR:O	1:A:973:LYS:CB	2.31	0.78
1:B:653:CYS:O	1:B:657:LEU:N	2.16	0.78
1:B:1101:GLN:O	1:B:1104:VAL:N	2.17	0.77
1:B:2060:ASN:O	1:B:2064:ILE:N	2.17	0.77
1:A:399:VAL:HA	1:A:420:THR:HA	1.66	0.77
1:A:853:PRO:O	1:A:855:SER:N	2.17	0.77
1:A:1285:SER:O	1:A:1341:VAL:CB	2.33	0.77
1:A:1839:GLN:O	1:A:1842:PHE:N	2.18	0.77
1:B:1625:LEU:O	1:B:1628:VAL:N	2.18	0.76
1:A:1794:VAL:CB	1:A:1831:LEU:O	2.33	0.76
1:B:666:ILE:CB	1:B:671:VAL:H	1.99	0.76
1:A:1839:GLN:O	1:A:1842:PHE:CB	2.33	0.76
1:B:2000:CYS:O	1:B:2003:LEU:N	2.17	0.76
1:A:1816:SER:O	1:A:1818:ARG:N	2.19	0.76
1:B:865:GLU:O	1:B:869:LEU:N	2.17	0.76
1:B:2090:ASN:O	1:B:2094:LEU:CB	2.34	0.76
1:A:101:LYS:O	1:A:104:GLU:N	2.19	0.76
1:A:1682:MET:CB	1:A:1686:ARG:CB	2.64	0.76
1:B:1178:GLU:O	1:B:1182:ARG:CB	2.34	0.76
1:B:140:ALA:N	1:B:146:ALA:O	2.19	0.75
1:A:977:ILE:O	1:A:981:ILE:N	2.18	0.75
1:B:1277:PHE:O	1:B:1280:ASN:N	2.20	0.75
1:B:1284:CYS:O	1:B:1286:GLU:N	2.19	0.74
1:B:1631:ARG:O	1:B:1634:LEU:N	2.20	0.74
1:A:1857:LYS:O	1:A:1859:PHE:N	2.20	0.74
1:A:1118:ASP:O	1:A:1119:LEU:C	2.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:TRP:HA	1:B:306:LYS:O	1.87	0.74
1:A:1048:THR:O	1:A:1050:LEU:N	2.20	0.74
1:A:1859:PHE:O	1:A:1862:ARG:N	2.21	0.74
1:B:1850:LYS:O	1:B:1851:LYS:C	2.31	0.74
1:B:2040:THR:O	1:B:2044:GLN:CB	2.36	0.74
1:A:898:VAL:C	1:A:900:VAL:HA	2.12	0.74
1:A:781:PHE:O	1:A:784:LEU:N	2.21	0.73
1:B:696:VAL:O	1:B:697:TRP:C	2.31	0.73
1:B:1286:GLU:O	1:B:1289:GLU:O	2.06	0.73
1:A:573:TYR:O	1:A:577:GLN:N	2.21	0.73
1:A:783:ARG:O	1:A:784:LEU:C	2.31	0.73
1:A:565:GLN:O	1:A:567:TYR:N	2.21	0.73
1:A:1194:VAL:O	1:A:1197:SER:N	2.22	0.73
1:B:2186:GLU:O	1:B:2189:ALA:N	2.21	0.73
1:B:125:HIS:O	1:B:129:ASN:N	2.21	0.73
1:A:769:SER:CB	1:A:779:ALA:HA	2.19	0.73
1:A:595:ILE:O	1:A:598:LEU:CB	2.37	0.72
1:B:1051:ASP:O	1:B:1055:HIS:N	2.21	0.72
1:A:782:CYS:O	1:A:785:MET:CB	2.37	0.72
1:A:2189:ALA:O	1:A:2191:HIS:N	2.22	0.72
1:B:1632:PRO:O	1:B:1635:LEU:N	2.23	0.72
1:A:1208:MET:O	1:A:1212:ALA:HB2	1.88	0.72
1:B:1682:MET:O	1:B:1685:ASP:C	2.33	0.72
1:A:2003:LEU:O	1:A:2007:ASP:N	2.17	0.72
1:B:2089:ASN:O	1:B:2093:LYS:CB	2.37	0.72
1:A:1802:GLY:O	1:A:1804:SER:N	2.22	0.71
1:B:1115:ILE:O	1:B:1117:GLN:N	2.23	0.71
1:B:684:GLU:O	1:B:687:LEU:N	2.24	0.71
1:B:2151:VAL:O	1:B:2155:ILE:N	2.21	0.71
1:A:565:GLN:C	1:A:567:TYR:H	1.97	0.71
1:B:1228:THR:HA	1:B:1271:VAL:CB	2.21	0.71
1:A:371:ASP:CB	1:A:389:ARG:O	2.39	0.71
1:B:740:PHE:O	1:B:742:ARG:N	2.24	0.71
1:B:2083:LEU:O	1:B:2086:GLU:N	2.24	0.70
1:B:1129:SER:O	1:B:1133:VAL:N	2.24	0.70
1:A:203:ASN:O	1:A:205:GLY:N	2.26	0.69
1:A:830:LYS:O	1:A:833:PHE:N	2.25	0.69
1:B:1632:PRO:O	1:B:1634:LEU:N	2.26	0.69
1:A:2075:PRO:O	1:A:2080:ARG:CB	2.40	0.69
1:B:1432:ASP:O	1:B:1493:PRO:C	2.36	0.69
1:B:894:ILE:O	1:B:897:CYS:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ALA:HB1	1:A:727:ARG:CB	2.23	0.69
1:A:1796:CYS:O	1:A:1800:LYS:N	2.23	0.68
1:B:971:LYS:O	1:B:974:ILE:N	2.19	0.68
1:B:984:VAL:O	1:B:989:ARG:N	2.26	0.68
1:A:1122:LEU:O	1:A:1125:ILE:N	2.26	0.68
1:A:1184:SER:O	1:A:1187:CYS:N	2.27	0.68
1:B:188:ASN:O	1:B:190:GLY:N	2.26	0.68
1:B:653:CYS:O	1:B:656:VAL:CB	2.42	0.68
1:A:852:PHE:O	1:A:856:ASP:CB	2.41	0.68
1:B:2149:ARG:O	1:B:2153:HIS:N	2.27	0.68
1:A:1807:VAL:O	1:A:1809:ASP:N	2.26	0.68
1:B:118:GLY:N	1:B:163:ILE:O	2.23	0.68
1:B:1115:ILE:C	1:B:1117:GLN:H	2.02	0.68
1:A:523:LEU:O	1:A:524:GLN:C	2.35	0.68
1:B:765:LEU:O	1:B:769:SER:N	2.23	0.68
1:B:1387:GLY:O	1:B:1389:ASN:N	2.27	0.68
1:A:1807:VAL:O	1:A:1808:ILE:C	2.37	0.68
1:A:725:GLU:O	1:A:729:ILE:N	2.20	0.68
1:A:1859:PHE:O	1:A:1860:TYR:C	2.36	0.68
1:A:1682:MET:O	1:A:1686:ARG:N	2.27	0.67
1:B:469:GLU:O	1:B:472:SER:N	2.28	0.67
1:B:1214:VAL:O	1:B:1216:GLU:N	2.28	0.67
1:B:1488:THR:O	1:B:1492:SER:N	2.27	0.67
1:B:1849:ASP:O	1:B:1850:LYS:C	2.38	0.67
1:B:1682:MET:O	1:B:1685:ASP:N	2.26	0.67
1:A:975:ILE:O	1:A:979:GLN:CB	2.43	0.67
1:A:1124:SER:O	1:A:1127:GLU:N	2.27	0.67
1:A:985:ARG:O	1:A:989:ARG:CB	2.43	0.67
1:B:862:LEU:O	1:B:863:THR:C	2.38	0.67
1:A:840:VAL:O	1:A:843:TYR:N	2.28	0.67
1:A:1378:VAL:O	1:A:1382:ALA:HB2	1.95	0.67
1:B:678:GLU:O	1:B:686:ALA:HB2	1.95	0.67
1:A:386:SER:O	1:A:432:ILE:N	2.17	0.67
1:A:856:ASP:O	1:A:860:ASN:CB	2.43	0.67
1:A:2083:LEU:O	1:A:2087:LEU:CB	2.42	0.66
1:A:1076:VAL:O	1:A:1079:ALA:HB3	1.96	0.66
1:B:694:GLU:O	1:B:696:VAL:C	2.38	0.66
1:A:997:PHE:O	1:A:999:ARG:N	2.27	0.66
1:B:1289:GLU:O	1:B:1291:VAL:N	2.27	0.66
1:B:1650:GLY:O	1:B:1653:CYS:N	2.29	0.66
1:A:1798:LEU:HA	1:A:1802:GLY:HA3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1212:ALA:O	1:B:1216:GLU:CB	2.43	0.66
1:A:125:HIS:O	1:A:129:ASN:CA	2.44	0.66
1:A:682:THR:O	1:A:686:ALA:HB3	1.96	0.66
1:A:1134:TYR:C	1:A:1230:MET:N	2.54	0.66
1:A:2189:ALA:O	1:A:2192:THR:N	2.29	0.66
1:B:628:PRO:O	1:B:632:ASP:N	2.21	0.66
1:B:1635:LEU:O	1:B:1639:ASN:CA	2.43	0.66
1:A:888:THR:O	1:A:891:LEU:CB	2.44	0.66
1:A:1371:LEU:O	1:A:1372:MET:C	2.39	0.66
1:B:1822:GLU:O	1:B:1826:LEU:N	2.25	0.66
1:B:2194:GLN:O	1:B:2196:GLU:N	2.27	0.66
1:A:1080:LEU:O	1:A:1083:LEU:CB	2.44	0.65
1:A:1623:SER:O	1:A:1626:VAL:N	2.29	0.65
1:A:783:ARG:O	1:A:786:LEU:N	2.29	0.65
1:A:1816:SER:C	1:A:1818:ARG:H	2.04	0.65
1:B:179:GLY:N	1:B:220:ILE:O	2.25	0.65
1:B:11:ILE:N	1:B:113:THR:O	2.25	0.65
1:B:972:LEU:O	1:B:976:GLU:CB	2.44	0.65
1:A:1224:LYS:HA	1:A:1270:ALA:HB3	1.77	0.65
1:A:1797:HIS:O	1:A:1798:LEU:C	2.39	0.65
1:A:1969:LEU:O	1:A:1972:LEU:N	2.30	0.65
1:B:1631:ARG:O	1:B:1632:PRO:C	2.40	0.65
1:A:1207:ASN:O	1:A:1210:ALA:N	2.29	0.65
1:B:857:LYS:O	1:B:858:GLU:C	2.39	0.65
1:A:387:TYR:HA	1:A:430:PHE:O	1.97	0.65
1:A:469:GLU:O	1:A:472:SER:N	2.29	0.65
1:A:789:HIS:O	1:A:791:ASP:N	2.29	0.65
1:B:285:GLU:O	1:B:303:PHE:HA	1.97	0.65
1:B:1813:ASN:C	1:B:1818:ARG:CB	2.70	0.65
1:A:864:PHE:O	1:A:865:GLU:C	2.36	0.65
1:A:1203:ARG:CB	1:A:1207:ASN:CB	2.74	0.65
1:B:552:ILE:O	1:B:555:LEU:CB	2.45	0.65
1:A:480:LEU:O	1:A:481:VAL:C	2.40	0.64
1:A:1273:MET:O	1:A:1276:ILE:N	2.31	0.64
1:B:1417:GLU:CB	1:B:1421:ALA:HB2	2.27	0.64
1:B:2188:TYR:O	1:B:2192:THR:CB	2.45	0.64
1:A:898:VAL:O	1:A:899:HIS:C	2.40	0.64
1:A:2168:GLU:O	1:A:2172:MET:CB	2.45	0.64
1:B:2068:LEU:O	1:B:2071:ASN:O	2.14	0.64
1:A:476:LEU:O	1:A:478:GLU:N	2.29	0.64
1:A:1973:GLN:O	1:A:1976:CYS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1635:LEU:HA	1:B:1646:CYS:CB	2.28	0.64
1:A:978:LEU:O	1:A:979:GLN:C	2.36	0.64
1:A:1208:MET:O	1:A:1212:ALA:HB3	1.96	0.64
1:A:2114:ASN:O	1:A:2116:ARG:N	2.30	0.64
1:B:1199:LYS:O	1:B:1202:GLN:N	2.31	0.64
1:B:1214:VAL:O	1:B:1215:LEU:C	2.39	0.64
1:B:1654:LYS:O	1:B:1655:LEU:C	2.41	0.64
1:A:2114:ASN:C	1:A:2116:ARG:N	2.54	0.64
1:B:833:PHE:O	1:B:836:THR:N	2.31	0.64
1:B:595:ILE:O	1:B:596:THR:C	2.39	0.64
1:B:893:ALA:O	1:B:894:ILE:C	2.40	0.64
1:A:2189:ALA:O	1:A:2193:ALA:N	2.20	0.64
1:B:766:ARG:O	1:B:768:MET:N	2.31	0.64
1:B:1649:GLY:O	1:B:1650:GLY:C	2.40	0.64
1:B:2083:LEU:O	1:B:2084:VAL:C	2.40	0.64
1:A:1417:GLU:O	1:A:1418:VAL:C	2.40	0.63
1:B:666:ILE:CB	1:B:670:LEU:H	2.10	0.63
1:B:841:GLU:O	1:B:844:LEU:N	2.30	0.63
1:B:1653:CYS:O	1:B:1656:ILE:N	2.31	0.63
1:A:1245:CYS:CB	1:A:1285:SER:O	2.46	0.63
1:B:985:ARG:O	1:B:989:ARG:CB	2.46	0.63
1:B:1289:GLU:C	1:B:1291:VAL:N	2.53	0.63
1:B:680:VAL:C	1:B:682:THR:N	2.51	0.63
1:A:588:ASP:CB	1:A:591:ALA:HB2	2.28	0.63
1:B:1634:LEU:O	1:B:1638:GLU:CB	2.47	0.63
1:A:1238:HIS:O	1:A:1240:PHE:N	2.32	0.63
1:A:844:LEU:O	1:A:847:VAL:CB	2.46	0.63
1:A:968:MET:O	1:A:971:LYS:CB	2.47	0.63
1:A:2119:GLU:O	1:A:2123:VAL:CB	2.47	0.63
1:B:682:THR:O	1:B:686:ALA:HB3	1.98	0.63
1:B:1225:ALA:HB1	1:B:1226:GLU:HA	1.81	0.63
1:B:1668:GLU:O	1:B:1671:CYS:N	2.31	0.63
1:A:707:ILE:O	1:A:709:SER:N	2.32	0.63
1:A:867:VAL:O	1:A:868:ASN:C	2.40	0.63
1:A:1859:PHE:O	1:A:1861:ASP:N	2.32	0.63
1:A:977:ILE:O	1:A:981:ILE:CB	2.47	0.62
1:A:1807:VAL:C	1:A:1809:ASP:N	2.54	0.62
1:B:842:GLU:O	1:B:845:ARG:N	2.32	0.62
1:B:680:VAL:C	1:B:682:THR:H	2.06	0.62
1:B:1313:GLN:O	1:B:1316:VAL:N	2.32	0.62
1:B:986:LEU:O	1:B:988:TYR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1638:GLU:O	1:B:1640:THR:CA	2.47	0.62
1:B:2088:LYS:O	1:B:2092:SER:N	2.31	0.62
1:B:2129:MET:O	1:B:2131:GLY:N	2.31	0.62
1:A:844:LEU:O	1:A:847:VAL:CA	2.47	0.62
1:B:1483:MET:CB	1:B:1886:LYS:CB	2.77	0.62
1:A:846:ASP:O	1:A:849:CYS:CB	2.48	0.62
1:A:1245:CYS:CB	1:A:1341:VAL:N	2.62	0.62
1:A:1833:GLY:C	1:A:1835:ASN:H	2.08	0.62
1:A:2189:ALA:C	1:A:2193:ALA:H	2.07	0.62
1:B:2000:CYS:O	1:B:2001:GLU:C	2.42	0.62
1:A:598:LEU:HA	1:A:602:ASN:CB	2.29	0.62
1:B:1231:GLN:HA	1:B:1275:HIS:CB	2.29	0.62
1:A:480:LEU:C	1:A:482:TYR:N	2.56	0.62
1:B:856:ASP:O	1:B:857:LYS:O	2.18	0.62
1:B:1086:HIS:O	1:B:1088:SER:N	2.32	0.62
1:A:1840:HIS:O	1:A:1841:SER:C	2.43	0.62
1:B:841:GLU:O	1:B:844:LEU:CB	2.48	0.62
1:A:269:ARG:HG3	2:A:3000:I3P:O4	2.00	0.62
1:A:888:THR:O	1:A:891:LEU:N	2.33	0.62
1:A:1134:TYR:O	1:A:1230:MET:N	2.33	0.62
1:B:593:ASP:O	1:B:594:THR:C	2.43	0.62
1:B:1222:TYR:CB	1:B:1272:THR:CB	2.77	0.62
1:B:1846:LEU:O	1:B:1853:GLU:CB	2.47	0.62
1:A:898:VAL:O	1:A:900:VAL:N	2.32	0.61
1:A:981:ILE:O	1:A:985:ARG:CB	2.48	0.61
1:B:2129:MET:O	1:B:2130:GLN:C	2.43	0.61
1:A:866:VAL:O	1:A:869:LEU:CB	2.48	0.61
1:A:1476:LYS:O	1:A:1479:THR:N	2.30	0.61
1:B:743:MET:HA	1:B:744:CYS:CB	2.30	0.61
1:B:1991:ASN:CB	1:B:1998:LEU:HA	2.30	0.61
1:A:626:ARG:C	1:A:628:PRO:N	2.56	0.61
1:A:1112:TYR:O	1:A:1115:ILE:N	2.33	0.61
1:A:715:LEU:O	1:A:716:ALA:C	2.42	0.61
1:A:1007:GLN:O	1:A:1009:SER:N	2.33	0.61
1:B:567:TYR:CE1	1:B:569:LYS:HB3	2.36	0.61
1:A:437:PRO:O	1:A:440:VAL:CB	2.49	0.61
1:B:576:LYS:C	1:B:578:PHE:N	2.58	0.61
1:B:588:ASP:C	1:B:590:LEU:N	2.57	0.61
1:B:1653:CYS:O	1:B:1654:LYS:C	2.43	0.61
1:A:1477:TYR:O	1:A:1481:ILE:CB	2.49	0.61
1:B:621:LEU:O	1:B:625:ASN:O	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1640:THR:CB	1:B:1646:CYS:CB	2.79	0.61
1:A:1842:PHE:O	1:A:1843:PHE:C	2.44	0.61
1:A:1857:LYS:C	1:A:1859:PHE:H	2.08	0.61
1:A:1798:LEU:CA	1:A:1802:GLY:HA3	2.31	0.61
1:B:2111:ILE:O	1:B:2112:LEU:C	2.44	0.61
1:B:622:VAL:O	1:B:626:ARG:HA	2.00	0.61
1:B:696:VAL:O	1:B:699:PHE:N	2.34	0.61
1:B:2150:ASN:O	1:B:2154:ASN:N	2.34	0.61
1:A:726:ASP:O	1:A:727:ARG:C	2.44	0.60
1:A:475:LYS:O	1:A:478:GLU:CB	2.48	0.60
1:A:769:SER:HA	1:A:773:LEU:CB	2.31	0.60
1:A:997:PHE:O	1:A:998:LYS:C	2.45	0.60
1:A:833:PHE:O	1:A:836:THR:CB	2.50	0.60
1:A:1422:TYR:O	1:A:1426:LEU:CB	2.49	0.60
1:B:2178:GLN:CB	1:B:2183:GLU:CB	2.79	0.60
1:A:967:VAL:O	1:A:968:MET:C	2.44	0.60
1:A:1081:GLN:O	1:A:1082:LEU:C	2.42	0.60
1:B:1650:GLY:O	1:B:1651:PHE:C	2.45	0.60
1:B:2110:ARG:O	1:B:2113:TYR:CB	2.49	0.60
1:A:704:ASN:C	1:A:706:GLU:H	2.09	0.60
1:A:885:LEU:O	1:A:888:THR:N	2.35	0.60
1:A:1795:GLN:HA	1:A:1798:LEU:CB	2.31	0.60
1:B:982:LEU:O	1:B:983:ASN:C	2.44	0.60
1:B:1449:LEU:O	1:B:1453:PHE:CB	2.49	0.60
1:A:625:ASN:CB	1:A:628:PRO:HA	2.32	0.60
1:A:2123:VAL:O	1:A:2127:ALA:HB3	2.02	0.60
1:B:782:CYS:O	1:B:785:MET:CB	2.50	0.60
1:B:1126:VAL:O	1:B:1129:SER:CB	2.49	0.60
1:A:1033:ILE:HA	1:A:1036:GLN:CB	2.32	0.60
1:A:1207:ASN:O	1:A:1209:GLY:N	2.35	0.60
1:A:1252:GLN:O	1:A:1256:HIS:CA	2.49	0.60
1:B:763:LEU:O	1:B:764:ILE:C	2.44	0.60
1:B:849:CYS:O	1:B:850:GLN:C	2.45	0.60
1:A:1222:TYR:CB	1:A:1272:THR:CB	2.80	0.60
1:B:682:THR:O	1:B:686:ALA:CB	2.50	0.60
1:B:742:ARG:CB	1:B:1040:ILE:CB	2.80	0.60
1:B:961:GLU:O	1:B:965:ILE:CB	2.50	0.60
1:B:982:LEU:O	1:B:984:VAL:N	2.35	0.60
1:B:232:ASP:O	1:B:384:ARG:N	2.29	0.60
1:B:766:ARG:C	1:B:768:MET:N	2.57	0.60
1:B:779:ALA:O	1:B:782:CYS:CB	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:LYS:O	1:B:977:ILE:CB	2.50	0.60
1:A:2076:LEU:CA	1:A:2080:ARG:CB	2.80	0.59
1:B:1631:ARG:O	1:B:1632:PRO:O	2.19	0.59
1:B:1798:LEU:HA	1:B:1802:GLY:N	2.17	0.59
1:B:1813:ASN:O	1:B:1815:SER:O	2.20	0.59
1:A:699:PHE:O	1:A:702:ASP:CB	2.50	0.59
1:A:974:ILE:O	1:A:975:ILE:C	2.44	0.59
1:A:1076:VAL:O	1:A:1080:LEU:N	2.26	0.59
1:B:1476:LYS:CB	1:B:1953:LYS:HA	2.32	0.59
1:A:988:TYR:O	1:A:989:ARG:C	2.45	0.59
1:B:893:ALA:O	1:B:896:ASP:N	2.35	0.59
1:A:998:LYS:O	1:A:1007:GLN:HA	2.02	0.59
1:A:1116:LYS:O	1:A:1117:GLN:C	2.44	0.59
1:A:1376:HIS:O	1:A:1380:LEU:CB	2.50	0.59
1:A:2150:ASN:O	1:A:2151:VAL:C	2.44	0.59
1:B:770:ASP:O	1:B:773:LEU:N	2.34	0.59
1:B:2197:ILE:HA	1:B:2212:PRO:CB	2.32	0.59
1:A:1194:VAL:O	1:A:1197:SER:CB	2.51	0.59
1:B:242:LEU:O	1:B:251:LEU:N	2.33	0.59
1:B:2044:GLN:C	1:B:2046:PRO:N	2.61	0.59
1:A:581:MET:O	1:A:585:ILE:CB	2.50	0.59
1:A:666:ILE:CB	1:A:670:LEU:N	2.66	0.59
1:A:870:ALA:HA	1:A:873:LEU:CB	2.31	0.59
1:A:1294:HIS:O	1:A:1298:CYS:CB	2.50	0.59
1:B:2161:GLN:O	1:B:2168:GLU:CB	2.50	0.59
1:B:684:GLU:O	1:B:687:LEU:CB	2.51	0.59
1:A:992:CYS:O	1:A:993:LEU:C	2.46	0.59
1:B:185:ASN:HA	1:B:192:PRO:CB	2.32	0.59
1:B:610:ILE:O	1:B:613:ALA:HB3	2.02	0.59
1:B:1640:THR:CB	1:B:1644:ARG:CB	2.81	0.59
1:B:1840:HIS:O	1:B:1841:SER:C	2.43	0.59
1:A:770:ASP:O	1:A:772:ASN:O	2.21	0.59
1:A:862:LEU:O	1:A:863:THR:C	2.45	0.59
1:A:1805:ASN:O	1:A:1808:ILE:N	2.36	0.59
1:B:981:ILE:O	1:B:985:ARG:CB	2.51	0.59
1:A:1954:ASP:O	1:A:1955:ASP:C	2.45	0.59
1:A:2032:ILE:O	1:A:2035:THR:N	2.36	0.59
1:A:980:PHE:O	1:A:981:ILE:C	2.45	0.58
1:A:2146:ALA:O	1:A:2148:PRO:N	2.35	0.58
1:B:894:ILE:O	1:B:895:LEU:C	2.45	0.58
1:B:1986:PHE:O	1:B:1988:ARG:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1862:ARG:O	1:A:1866:ALA:HB2	2.02	0.58
1:B:1833:GLY:C	1:B:1835:ASN:H	2.11	0.58
1:B:2202:ARG:CB	1:B:2206:GLN:HA	2.33	0.58
1:B:666:ILE:CB	1:B:667:GLU:C	2.76	0.58
1:B:105:THR:O	1:B:106:GLU:C	2.45	0.58
1:B:588:ASP:CB	1:B:591:ALA:H	2.15	0.58
1:B:621:LEU:O	1:B:622:VAL:C	2.46	0.58
1:B:1850:LYS:O	1:B:1854:LYS:CB	2.52	0.58
1:B:2189:ALA:O	1:B:2193:ALA:HB3	2.04	0.58
1:A:2019:LEU:O	1:A:2021:GLY:N	2.37	0.58
1:B:679:GLY:O	1:B:681:SER:N	2.37	0.58
1:B:871:ARG:O	1:B:872:ASN:C	2.47	0.58
1:B:982:LEU:O	1:B:985:ARG:N	2.37	0.58
1:A:243:PHE:O	1:A:430:PHE:HA	2.04	0.58
1:A:777:LEU:O	1:A:780:SER:CB	2.51	0.58
1:A:1215:LEU:O	1:A:1217:LEU:N	2.37	0.58
1:A:1251:ASN:CB	1:A:1283:LEU:HA	2.33	0.58
1:A:1860:TYR:O	1:A:1863:MET:N	2.35	0.58
1:B:1636:PHE:O	1:B:1638:GLU:N	2.36	0.58
1:A:1813:ASN:CB	1:A:1821:HIS:CB	2.82	0.58
1:A:1839:GLN:O	1:A:1840:HIS:C	2.47	0.58
1:B:2185:LEU:HA	1:B:2188:TYR:CB	2.33	0.58
1:A:781:PHE:O	1:A:783:ARG:N	2.36	0.58
1:A:1252:GLN:O	1:A:1256:HIS:CB	2.51	0.58
1:B:140:ALA:HB3	1:B:143:GLU:O	2.03	0.58
1:B:188:ASN:C	1:B:190:GLY:N	2.62	0.58
1:B:748:GLN:O	1:B:749:TYR:CB	2.52	0.58
1:B:2087:LEU:O	1:B:2091:ALA:CB	2.51	0.58
1:A:676:GLU:O	1:A:679:GLY:N	2.37	0.57
1:B:666:ILE:CB	1:B:670:LEU:N	2.67	0.57
1:B:1093:VAL:HA	1:B:1176:VAL:N	2.19	0.57
1:B:2203:THR:O	1:B:2204:MET:CB	2.51	0.57
1:A:682:THR:C	1:A:686:ALA:HB3	2.29	0.57
1:A:749:TYR:O	1:A:751:ALA:N	2.37	0.57
1:A:860:ASN:O	1:A:861:LYS:C	2.46	0.57
1:B:681:SER:O	1:B:682:THR:C	2.45	0.57
1:B:985:ARG:O	1:B:989:ARG:N	2.37	0.57
1:B:1863:MET:O	1:B:1864:LYS:C	2.46	0.57
1:A:1076:VAL:HA	1:A:1079:ALA:CB	2.34	0.57
1:A:1197:SER:O	1:A:1200:GLN:N	2.37	0.57
1:A:1864:LYS:O	1:A:1865:VAL:C	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1998:LEU:C	1:A:2000:CYS:H	2.12	0.57
1:A:1998:LEU:C	1:A:2000:CYS:N	2.60	0.57
1:B:737:LEU:O	1:B:739:LEU:N	2.36	0.57
1:A:520:PHE:C	1:A:522:LEU:H	2.12	0.57
1:B:1682:MET:C	1:B:1686:ARG:H	2.12	0.57
1:B:1287:ILE:O	1:B:1288:ASN:CB	2.52	0.57
1:B:1289:GLU:O	1:B:1290:ARG:C	2.47	0.57
1:A:263:PHE:HA	1:A:416:LEU:O	2.05	0.57
1:B:469:GLU:O	1:B:471:ARG:N	2.37	0.57
1:A:969:ASP:O	1:A:970:THR:C	2.44	0.57
1:A:681:SER:O	1:A:682:THR:O	2.23	0.57
1:A:781:PHE:C	1:A:783:ARG:N	2.61	0.57
1:B:1827:ALA:O	1:B:1828:ILE:C	2.47	0.57
1:B:1843:PHE:O	1:B:1846:LEU:N	2.37	0.57
1:B:985:ARG:HA	1:B:989:ARG:CB	2.34	0.57
1:A:503:ASN:O	1:A:507:GLN:HG3	2.04	0.56
1:A:653:CYS:O	1:A:656:VAL:CB	2.53	0.56
1:B:775:TYR:O	1:B:776:ASP:CB	2.53	0.56
1:B:969:ASP:O	1:B:970:THR:C	2.47	0.56
1:B:974:ILE:O	1:B:978:LEU:CB	2.53	0.56
1:B:1240:PHE:CB	1:B:1244:PHE:O	2.53	0.56
1:B:2193:ALA:O	1:B:2195:ILE:N	2.35	0.56
1:A:753:ASN:O	1:A:754:GLU:C	2.48	0.56
1:A:770:ASP:O	1:A:771:GLU:C	2.48	0.56
1:A:850:GLN:O	1:A:851:ARG:C	2.48	0.56
1:A:978:LEU:O	1:A:982:LEU:CB	2.54	0.56
1:A:1061:LEU:HA	1:A:1101:GLN:CB	2.35	0.56
1:A:1178:GLU:O	1:A:1182:ARG:CB	2.53	0.56
1:A:1477:TYR:HA	1:A:1881:LEU:C	2.31	0.56
1:B:14:ILE:HA	1:B:58:PHE:O	2.05	0.56
1:B:282:TRP:CA	1:B:306:LYS:O	2.53	0.56
1:B:976:GLU:O	1:B:978:LEU:N	2.38	0.56
1:B:1052:LEU:O	1:B:1057:GLY:N	2.39	0.56
1:B:1798:LEU:HA	1:B:1802:GLY:CA	2.35	0.56
1:A:474:THR:O	1:A:475:LYS:C	2.48	0.56
1:A:708:ARG:H	1:A:711:SER:CB	2.18	0.56
1:A:768:MET:O	1:A:772:ASN:C	2.48	0.56
1:A:2194:GLN:N	1:A:2216:GLU:CB	2.68	0.56
1:B:753:ASN:O	1:B:756:SER:CB	2.54	0.56
1:B:1651:PHE:O	1:B:1652:ILE:C	2.48	0.56
1:B:1815:SER:O	1:B:1816:SER:C	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:GLU:O	1:A:689:ALA:C	2.48	0.56
1:A:1863:MET:O	1:A:1867:GLN:CB	2.54	0.56
1:B:1245:CYS:CB	1:B:1285:SER:CB	2.82	0.56
1:B:503:ASN:O	1:B:507:GLN:HG3	2.06	0.56
1:A:519:ILE:O	1:A:522:LEU:N	2.34	0.56
1:A:552:ILE:O	1:A:555:LEU:CB	2.54	0.56
1:B:1657:LYS:O	1:B:1660:LYS:N	2.33	0.56
1:A:475:LYS:O	1:A:476:LEU:C	2.49	0.56
1:A:588:ASP:C	1:A:590:LEU:N	2.62	0.56
1:A:781:PHE:O	1:A:782:CYS:C	2.49	0.56
1:A:978:LEU:O	1:A:979:GLN:O	2.24	0.56
1:A:1846:LEU:O	1:A:1847:THR:C	2.45	0.56
1:B:1230:MET:O	1:B:1234:MET:CB	2.54	0.56
1:B:1652:ILE:O	1:B:1653:CYS:C	2.49	0.56
1:A:683:GLY:O	1:A:684:GLU:C	2.49	0.56
1:A:873:LEU:O	1:A:874:ILE:C	2.49	0.56
1:A:1679:ARG:O	1:A:1682:MET:CB	2.53	0.56
1:A:1998:LEU:O	1:A:2000:CYS:N	2.39	0.56
1:B:743:MET:CA	1:B:744:CYS:CB	2.84	0.56
1:B:867:VAL:O	1:B:868:ASN:C	2.48	0.56
1:A:15:CYS:CB	1:A:222:LEU:HA	2.36	0.55
1:A:1377:LEU:C	1:A:1381:LEU:H	2.15	0.55
1:A:1682:MET:HA	1:A:1686:ARG:H	1.71	0.55
1:A:2185:LEU:HA	1:A:2188:TYR:CB	2.36	0.55
1:B:848:VAL:O	1:B:850:GLN:N	2.39	0.55
1:B:2049:GLU:O	1:B:2053:CYS:CB	2.54	0.55
1:A:476:LEU:C	1:A:478:GLU:N	2.58	0.55
1:A:1061:LEU:O	1:A:1065:LEU:N	2.31	0.55
1:A:1188:VAL:O	1:A:1191:SER:N	2.39	0.55
1:A:1209:GLY:O	1:A:1213:VAL:CB	2.54	0.55
1:B:869:LEU:O	1:B:870:ALA:C	2.48	0.55
1:B:1682:MET:C	1:B:1686:ARG:N	2.62	0.55
1:A:469:GLU:O	1:A:470:ARG:C	2.48	0.55
1:A:763:LEU:O	1:A:764:ILE:C	2.49	0.55
1:A:845:ARG:O	1:A:848:VAL:N	2.39	0.55
1:A:899:HIS:N	1:A:900:VAL:HA	2.21	0.55
1:B:549:PHE:C	1:B:551:HIS:N	2.63	0.55
1:B:750:LEU:O	1:B:751:ALA:C	2.48	0.55
1:B:856:ASP:O	1:B:860:ASN:N	2.29	0.55
1:B:1228:THR:CB	1:B:1271:VAL:CB	2.85	0.55
1:B:1851:LYS:O	1:B:1855:PHE:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2060:ASN:O	1:A:2061:GLY:C	2.49	0.55
1:B:615:ILE:O	1:B:616:ASP:C	2.48	0.55
1:B:782:CYS:O	1:B:785:MET:CA	2.54	0.55
1:B:986:LEU:C	1:B:988:TYR:N	2.64	0.55
1:B:2001:GLU:O	1:B:2004:GLN:N	2.39	0.55
1:A:565:GLN:C	1:A:567:TYR:N	2.65	0.55
1:A:650:GLU:O	1:A:651:LEU:C	2.49	0.55
1:B:729:ILE:O	1:B:732:TYR:CB	2.55	0.55
1:B:854:PHE:O	1:B:857:LYS:CB	2.55	0.55
1:A:598:LEU:O	1:A:599:LEU:C	2.49	0.55
1:A:867:VAL:HA	1:A:870:ALA:HB3	1.89	0.55
1:A:1096:ALA:O	1:A:1100:VAL:N	2.39	0.55
1:B:1251:ASN:CB	1:B:1283:LEU:HA	2.37	0.55
1:B:1966:GLN:C	1:B:1970:ARG:H	2.15	0.55
1:B:2133:VAL:O	1:B:2134:GLU:C	2.47	0.55
1:B:1327:GLN:O	1:B:1330:VAL:CB	2.54	0.55
1:B:692:ASP:O	1:B:693:GLU:C	2.49	0.55
1:B:842:GLU:O	1:B:843:TYR:C	2.48	0.55
1:A:776:ASP:O	1:A:777:LEU:C	2.49	0.54
1:A:777:LEU:O	1:A:780:SER:N	2.40	0.54
1:A:1335:VAL:O	1:A:1384:CYS:CB	2.55	0.54
1:A:2003:LEU:O	1:A:2007:ASP:CB	2.55	0.54
1:B:567:TYR:CD2	1:B:570:ASN:HB2	2.42	0.54
1:A:69:GLN:HA	1:A:96:ALA:CB	2.36	0.54
1:A:2131:GLY:HA3	1:A:2147:SER:CB	2.37	0.54
1:B:588:ASP:CB	1:B:591:ALA:N	2.71	0.54
1:B:1489:PHE:HA	1:B:1493:PRO:HA	1.89	0.54
1:B:1623:SER:O	1:B:1626:VAL:CB	2.55	0.54
1:B:1986:PHE:O	1:B:1987:LEU:C	2.50	0.54
1:A:773:LEU:CB	1:A:778:ARG:CB	2.85	0.54
1:A:1129:SER:CB	1:A:1180:LEU:HA	2.37	0.54
1:A:1345:TYR:O	1:A:1350:SER:CB	2.55	0.54
1:A:1627:ASP:O	1:A:1630:HIS:N	2.41	0.54
1:B:991:SER:O	1:B:994:LEU:CB	2.55	0.54
1:A:2122:GLU:O	1:A:2126:LYS:CB	2.55	0.54
1:B:235:LYS:O	1:B:236:GLY:C	2.50	0.54
1:B:666:ILE:CB	1:B:668:THR:C	2.81	0.54
1:B:694:GLU:O	1:B:695:GLU:C	2.50	0.54
1:B:1053:ASP:O	1:B:1057:GLY:HA3	2.08	0.54
1:B:1459:ARG:C	1:B:1461:CYS:H	2.15	0.54
1:B:1682:MET:C	1:B:1685:ASP:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2001:GLU:O	1:B:2002:THR:C	2.51	0.54
1:A:710:LYS:HA	1:A:713:ARG:CB	2.38	0.54
1:A:783:ARG:C	1:A:785:MET:N	2.63	0.54
1:A:976:GLU:HA	1:A:979:GLN:CB	2.37	0.54
1:B:590:LEU:O	1:B:593:ASP:N	2.35	0.54
1:B:2184:ALA:O	1:B:2188:TYR:CB	2.55	0.54
1:A:573:TYR:O	1:A:577:GLN:CB	2.55	0.54
1:A:891:LEU:O	1:A:892:LEU:C	2.49	0.54
1:B:549:PHE:O	1:B:550:ARG:C	2.50	0.54
1:B:871:ARG:C	1:B:873:LEU:N	2.65	0.54
1:B:873:LEU:O	1:B:874:ILE:C	2.46	0.54
1:B:2015:GLY:O	1:B:2067:ALA:HB1	2.07	0.54
1:B:2082:ASP:O	1:B:2083:LEU:C	2.48	0.54
1:A:666:ILE:CB	1:A:667:GLU:C	2.80	0.54
1:A:742:ARG:O	1:A:743:MET:C	2.50	0.54
1:B:188:ASN:C	1:B:190:GLY:H	2.15	0.54
1:B:473:VAL:O	1:B:474:THR:C	2.47	0.54
1:B:652:ILE:O	1:B:655:ALA:HB3	2.08	0.54
1:B:786:LEU:O	1:B:789:HIS:N	2.40	0.54
1:B:1042:GLY:O	1:B:1043:GLY:C	2.50	0.54
1:B:1275:HIS:O	1:B:1279:ASN:CB	2.56	0.54
1:B:1403:ASP:HA	1:B:1406:VAL:CB	2.38	0.54
1:A:838:GLU:O	1:A:841:GLU:N	2.41	0.54
1:B:510:MET:SD	1:B:515:ILE:CB	2.96	0.54
1:B:707:ILE:CB	1:B:1046:GLU:CB	2.85	0.54
1:B:1225:ALA:HA	1:B:1226:GLU:C	2.32	0.54
1:B:1625:LEU:O	1:B:1628:VAL:CB	2.56	0.54
1:A:268:GLY:CA	2:A:3000:I3P:O42	2.55	0.54
1:A:780:SER:O	1:A:783:ARG:CB	2.55	0.54
1:A:1476:LYS:CB	1:A:1883:ASN:HA	2.38	0.54
1:B:1379:GLU:O	1:B:1382:ALA:HB3	2.08	0.54
1:A:1076:VAL:HA	1:A:1079:ALA:HB3	1.89	0.54
1:B:678:GLU:O	1:B:680:VAL:O	2.26	0.54
1:B:998:LYS:O	1:B:999:ARG:CB	2.56	0.54
1:B:1191:SER:CB	1:B:1236:LEU:O	2.56	0.54
1:A:1636:PHE:O	1:A:1638:GLU:N	2.41	0.53
1:A:1679:ARG:HA	1:A:1682:MET:CB	2.38	0.53
1:A:1847:THR:O	1:A:1848:GLU:C	2.51	0.53
1:B:1094:LEU:O	1:B:1095:GLN:C	2.50	0.53
1:B:1378:VAL:O	1:B:1382:ALA:HB2	2.08	0.53
1:A:564:GLN:O	1:A:571:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:LEU:O	1:A:751:ALA:C	2.51	0.53
1:A:897:CYS:C	1:A:899:HIS:H	2.14	0.53
1:A:1972:LEU:O	1:A:1975:LEU:CB	2.56	0.53
1:B:590:LEU:O	1:B:592:GLU:N	2.40	0.53
1:A:1371:LEU:O	1:A:1374:HIS:N	2.41	0.53
1:B:678:GLU:CB	1:B:686:ALA:HA	2.38	0.53
1:B:769:SER:O	1:B:773:LEU:HA	2.08	0.53
1:B:2190:LYS:O	1:B:2195:ILE:CB	2.56	0.53
1:A:743:MET:O	1:A:744:CYS:C	2.50	0.53
1:A:1316:VAL:HA	1:A:1319:GLU:CB	2.38	0.53
1:A:1820:PHE:O	1:A:1823:SER:N	2.42	0.53
1:B:1238:HIS:O	1:B:1240:PHE:N	2.42	0.53
1:B:1277:PHE:O	1:B:1278:MET:C	2.51	0.53
1:A:1817:ASP:O	1:A:1818:ARG:C	2.51	0.53
1:B:729:ILE:O	1:B:732:TYR:N	2.42	0.53
1:B:1193:SER:C	1:B:1197:SER:CB	2.82	0.53
1:B:2182:ASP:C	1:B:2184:ALA:N	2.65	0.53
1:A:1476:LYS:CB	1:A:1884:LYS:HA	2.39	0.53
1:A:1807:VAL:C	1:A:1809:ASP:H	2.16	0.53
1:B:870:ALA:O	1:B:874:ILE:N	2.37	0.53
1:B:1377:LEU:O	1:B:1381:LEU:CB	2.57	0.53
1:B:1823:SER:O	1:B:1824:ILE:C	2.48	0.53
1:B:2111:ILE:C	1:B:2113:TYR:N	2.63	0.53
1:B:594:THR:O	1:B:597:ALA:HB3	2.09	0.53
1:B:1290:ARG:O	1:B:1291:VAL:C	2.52	0.53
1:A:751:ALA:O	1:A:752:ILE:C	2.52	0.53
1:A:1654:LYS:O	1:A:1656:ILE:N	2.42	0.53
1:A:1839:GLN:O	1:A:1842:PHE:CA	2.57	0.53
1:A:1842:PHE:O	1:A:1845:ARG:N	2.42	0.53
1:B:1093:VAL:O	1:B:1095:GLN:N	2.42	0.53
1:B:707:ILE:O	1:B:708:ARG:CB	2.57	0.53
1:A:772:ASN:O	1:A:774:PRO:N	2.41	0.53
1:A:863:THR:O	1:A:866:VAL:CB	2.57	0.53
1:A:1287:ILE:HA	1:A:1344:PHE:CB	2.38	0.53
1:A:1295:PHE:C	1:A:1297:HIS:N	2.65	0.53
1:A:1638:GLU:O	1:A:1639:ASN:C	2.52	0.53
1:A:1809:ASP:O	1:A:1811:ILE:N	2.42	0.53
1:A:2189:ALA:O	1:A:2190:LYS:C	2.51	0.53
1:B:111:LEU:C	1:B:113:THR:H	2.18	0.53
1:B:778:ARG:O	1:B:779:ALA:C	2.51	0.53
1:B:781:PHE:O	1:B:784:LEU:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:PHE:O	1:B:551:HIS:N	2.43	0.52
1:A:645:ILE:O	1:A:646:PRO:C	2.50	0.52
1:A:724:LYS:C	1:A:726:ASP:H	2.17	0.52
1:A:1817:ASP:O	1:A:1821:HIS:CB	2.57	0.52
1:B:697:TRP:O	1:B:698:LEU:C	2.50	0.52
1:A:181:LYS:HA	1:A:218:TRP:O	2.10	0.52
1:A:707:ILE:C	1:A:711:SER:H	2.17	0.52
1:A:883:ASP:C	1:A:885:LEU:N	2.66	0.52
1:A:1679:ARG:C	1:A:1682:MET:H	2.16	0.52
1:A:1809:ASP:O	1:A:1810:LEU:C	2.52	0.52
1:B:590:LEU:C	1:B:592:GLU:N	2.67	0.52
1:B:620:SER:O	1:B:621:LEU:C	2.53	0.52
1:B:1194:VAL:N	1:B:1197:SER:CB	2.72	0.52
1:B:2092:SER:O	1:B:2096:LEU:CB	2.57	0.52
1:A:769:SER:O	1:A:773:LEU:CB	2.58	0.52
1:A:1868:GLN:O	1:A:1869:GLU:C	2.52	0.52
1:B:621:LEU:O	1:B:625:ASN:C	2.52	0.52
1:B:1638:GLU:O	1:B:1640:THR:CB	2.58	0.52
1:B:2061:GLY:O	1:B:2062:ILE:C	2.52	0.52
1:A:692:ASP:O	1:A:693:GLU:C	2.52	0.52
1:A:1245:CYS:CB	1:A:1285:SER:CB	2.88	0.52
1:A:1859:PHE:C	1:A:1861:ASP:N	2.65	0.52
1:B:200:LEU:N	1:B:206:CYS:O	2.43	0.52
1:B:1310:LYS:O	1:B:1311:PHE:CB	2.57	0.52
1:A:769:SER:O	1:A:772:ASN:O	2.27	0.52
1:A:1085:ARG:O	1:A:1087:PHE:N	2.43	0.52
1:B:870:ALA:O	1:B:873:LEU:CB	2.58	0.52
1:B:2053:CYS:O	1:B:2054:ILE:C	2.52	0.52
1:A:1317:LYS:CA	1:A:1323:ILE:CB	2.86	0.52
1:A:1612:ASP:O	1:A:1613:ARG:C	2.53	0.52
1:B:106:GLU:O	1:B:109:LYS:N	2.36	0.52
1:B:868:ASN:O	1:B:869:LEU:C	2.53	0.52
1:B:976:GLU:C	1:B:978:LEU:N	2.64	0.52
1:B:1223:GLU:O	1:B:1270:ALA:C	2.52	0.52
1:B:1632:PRO:O	1:B:1633:GLU:C	2.52	0.52
1:A:830:LYS:O	1:A:833:PHE:CB	2.58	0.52
1:A:979:GLN:O	1:A:980:PHE:C	2.50	0.52
1:A:1628:VAL:O	1:A:1629:LEU:C	2.51	0.52
1:B:785:MET:O	1:B:786:LEU:C	2.52	0.52
1:B:1682:MET:CB	1:B:1686:ARG:H	2.23	0.52
1:B:2152:GLY:O	1:B:2156:TYR:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:ARG:O	1:A:767:CYS:C	2.52	0.52
1:A:983:ASN:O	1:A:984:VAL:C	2.53	0.52
1:A:1071:ASP:O	1:A:1072:TYR:C	2.52	0.52
1:A:984:VAL:O	1:A:985:ARG:C	2.53	0.51
1:B:269:ARG:NH2	2:B:3000:I3P:O51	2.34	0.51
1:B:2129:MET:O	1:B:2132:GLU:N	2.42	0.51
1:A:412:LYS:CB	1:A:1257:LYS:CB	2.88	0.51
1:A:1654:LYS:C	1:A:1656:ILE:N	2.63	0.51
1:A:1791:LEU:O	1:A:1795:GLN:CB	2.58	0.51
1:B:1489:PHE:HA	1:B:1493:PRO:C	2.36	0.51
1:B:1826:LEU:O	1:B:1827:ALA:C	2.50	0.51
1:A:553:CYS:C	1:A:555:LEU:H	2.16	0.51
1:A:2178:GLN:CB	1:A:2183:GLU:CB	2.88	0.51
1:B:1093:VAL:O	1:B:1094:LEU:C	2.54	0.51
1:B:1193:SER:CB	1:B:1197:SER:CB	2.88	0.51
1:B:1682:MET:CB	1:B:1687:GLY:H	2.23	0.51
1:B:2086:GLU:O	1:B:2090:ASN:CB	2.58	0.51
1:A:683:GLY:O	1:A:685:ASN:N	2.44	0.51
1:A:708:ARG:O	1:A:712:VAL:CA	2.58	0.51
1:A:761:VAL:O	1:A:762:ASP:C	2.53	0.51
1:A:1007:GLN:C	1:A:1009:SER:H	2.16	0.51
1:A:2020:LEU:O	1:A:2024:ILE:CA	2.52	0.51
1:A:2150:ASN:O	1:A:2152:GLY:N	2.44	0.51
1:A:2150:ASN:C	1:A:2152:GLY:N	2.66	0.51
1:B:469:GLU:C	1:B:471:ARG:N	2.65	0.51
1:B:829:ILE:O	1:B:832:ARG:N	2.44	0.51
1:B:885:LEU:C	1:B:888:THR:H	2.16	0.51
1:A:778:ARG:O	1:A:779:ALA:C	2.49	0.51
1:A:978:LEU:HA	1:A:981:ILE:CB	2.40	0.51
1:B:568:ARG:O	1:B:572:GLU:HG3	2.11	0.51
1:B:892:LEU:O	1:B:893:ALA:O	2.29	0.51
1:B:986:LEU:C	1:B:988:TYR:H	2.19	0.51
1:A:1095:GLN:O	1:A:1096:ALA:C	2.54	0.51
1:B:1210:ALA:O	1:B:1211:HIS:C	2.53	0.51
1:B:1246:ALA:O	1:B:1248:ASN:N	2.43	0.51
1:B:1640:THR:CB	1:B:1644:ARG:O	2.59	0.51
1:A:118:GLY:N	1:A:163:ILE:O	2.42	0.51
1:A:867:VAL:O	1:A:871:ARG:CB	2.59	0.51
1:A:874:ILE:O	1:A:878:PHE:N	2.43	0.51
1:B:101:LYS:O	1:B:104:GLU:N	2.44	0.51
1:B:1201:GLN:C	1:B:1203:ARG:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1630:HIS:O	1:B:1631:ARG:C	2.54	0.51
1:B:1813:ASN:O	1:B:1814:ALA:C	2.54	0.51
1:B:2186:GLU:O	1:B:2189:ALA:HB3	2.11	0.51
1:A:250:PHE:O	1:A:264:LEU:HA	2.11	0.51
1:A:476:LEU:O	1:A:478:GLU:C	2.53	0.51
1:A:1295:PHE:C	1:A:1297:HIS:H	2.19	0.51
1:A:2150:ASN:C	1:A:2153:HIS:H	2.13	0.51
1:B:199:GLN:HA	1:B:206:CYS:O	2.11	0.51
1:B:252:THR:O	1:B:262:VAL:HA	2.10	0.51
1:B:1231:GLN:CB	1:B:1275:HIS:CB	2.89	0.51
1:B:1315:ILE:O	1:B:1316:VAL:C	2.52	0.51
1:A:476:LEU:O	1:A:477:LEU:C	2.54	0.51
1:B:858:GLU:O	1:B:859:LYS:C	2.52	0.51
1:B:1214:VAL:O	1:B:1217:LEU:N	2.35	0.51
1:B:1354:LEU:O	1:B:1355:ILE:C	2.54	0.51
1:B:1489:PHE:HA	1:B:1493:PRO:CA	2.41	0.51
1:B:2186:GLU:O	1:B:2187:PHE:C	2.54	0.51
1:A:829:ILE:O	1:A:830:LYS:C	2.54	0.51
1:A:976:GLU:O	1:A:977:ILE:C	2.52	0.51
1:B:52:LYS:O	1:B:54:ARG:N	2.43	0.51
1:B:721:GLU:O	1:B:722:GLY:C	2.53	0.51
1:B:984:VAL:O	1:B:985:ARG:C	2.53	0.51
1:B:1376:HIS:C	1:B:1378:VAL:H	2.19	0.51
1:A:125:HIS:O	1:A:129:ASN:HA	2.11	0.50
1:A:830:LYS:O	1:A:831:GLU:C	2.54	0.50
1:A:970:THR:HA	1:A:973:LYS:CB	2.41	0.50
1:B:576:LYS:C	1:B:578:PHE:H	2.19	0.50
1:B:469:GLU:O	1:B:470:ARG:C	2.55	0.50
1:B:841:GLU:O	1:B:842:GLU:C	2.52	0.50
1:A:559:VAL:O	1:A:562:HIS:CB	2.59	0.50
1:A:1213:VAL:HA	1:A:1216:GLU:CB	2.41	0.50
1:B:978:LEU:O	1:B:979:GLN:C	2.52	0.50
1:B:1813:ASN:O	1:B:1818:ARG:CB	2.58	0.50
1:B:1850:LYS:O	1:B:1852:SER:N	2.44	0.50
1:A:666:ILE:CB	1:A:671:VAL:H	2.25	0.50
1:A:1218:LEU:O	1:A:1221:PRO:O	2.30	0.50
1:B:552:ILE:O	1:B:555:LEU:CA	2.59	0.50
1:B:1061:LEU:O	1:B:1062:ARG:C	2.53	0.50
1:B:1190:GLU:O	1:B:1193:SER:CB	2.60	0.50
1:B:1816:SER:O	1:B:1817:ASP:CB	2.59	0.50
1:A:2035:THR:O	1:A:2039:LEU:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1101:GLN:O	1:B:1102:LEU:C	2.53	0.50
1:B:1293:GLN:CB	1:B:1345:TYR:O	2.59	0.50
1:B:1650:GLY:O	1:B:1653:CYS:CB	2.59	0.50
1:B:1973:GLN:O	1:B:1976:CYS:N	2.45	0.50
1:B:2014:THR:O	1:B:2067:ALA:HB2	2.11	0.50
1:A:588:ASP:O	1:A:591:ALA:HB3	2.11	0.50
1:A:1476:LYS:C	1:A:1478:VAL:N	2.69	0.50
1:B:611:THR:C	1:B:613:ALA:N	2.69	0.50
1:A:1848:GLU:C	1:A:1850:LYS:H	2.20	0.50
1:B:282:TRP:CB	1:B:306:LYS:O	2.60	0.50
1:B:761:VAL:O	1:B:762:ASP:C	2.55	0.50
1:B:971:LYS:O	1:B:972:LEU:C	2.54	0.50
1:B:1293:GLN:HA	1:B:1345:TYR:HA	1.92	0.50
1:B:1640:THR:CB	1:B:1644:ARG:C	2.85	0.50
1:A:2146:ALA:O	1:A:2150:ASN:CB	2.59	0.50
1:B:666:ILE:CB	1:B:668:THR:N	2.75	0.50
1:B:888:THR:O	1:B:891:LEU:N	2.44	0.50
1:B:967:VAL:C	1:B:969:ASP:N	2.70	0.50
1:B:1096:ALA:O	1:B:1097:PHE:C	2.51	0.50
1:B:1313:GLN:O	1:B:1314:THR:C	2.54	0.50
1:A:660:THR:O	1:A:662:ALA:N	2.45	0.50
1:A:1061:LEU:O	1:A:1064:LEU:CB	2.60	0.50
1:B:766:ARG:C	1:B:768:MET:H	2.19	0.50
1:B:992:CYS:O	1:B:993:LEU:C	2.53	0.50
1:B:1470:ALA:O	1:B:1471:ASP:CB	2.60	0.50
1:A:628:PRO:O	1:A:631:LEU:CB	2.59	0.49
1:A:1194:VAL:O	1:A:1195:ARG:C	2.55	0.49
1:B:832:ARG:O	1:B:833:PHE:C	2.54	0.49
1:B:1682:MET:CA	1:B:1686:ARG:H	2.25	0.49
1:B:1798:LEU:O	1:B:1801:GLU:N	2.45	0.49
1:A:758:GLN:O	1:A:759:LEU:C	2.54	0.49
1:A:1612:ASP:O	1:A:1615:ARG:N	2.45	0.49
1:A:2062:ILE:O	1:A:2063:ASP:C	2.55	0.49
1:B:316:ALA:HA	1:B:354:SER:O	2.12	0.49
1:B:974:ILE:O	1:B:975:ILE:C	2.53	0.49
1:B:992:CYS:C	1:B:994:LEU:N	2.69	0.49
1:B:1292:VAL:O	1:B:1295:PHE:CB	2.60	0.49
1:B:1825:LEU:O	1:B:1826:LEU:C	2.53	0.49
1:A:117:TYR:HA	1:A:163:ILE:O	2.12	0.49
1:A:392:HIS:O	1:A:396:ASN:N	2.45	0.49
1:A:707:ILE:HA	1:A:710:LYS:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:CYS:O	1:A:994:LEU:N	2.45	0.49
1:A:1191:SER:CB	1:A:1236:LEU:O	2.61	0.49
1:B:762:ASP:O	1:B:766:ARG:N	2.24	0.49
1:B:773:LEU:C	1:B:775:TYR:N	2.70	0.49
1:B:885:LEU:O	1:B:886:ARG:C	2.52	0.49
1:A:748:GLN:CB	1:A:1074:PRO:CB	2.90	0.49
1:A:1280:ASN:O	1:A:1281:PHE:C	2.55	0.49
1:A:1605:ASP:O	1:A:1609:ALA:HB2	2.11	0.49
1:B:1215:LEU:O	1:B:1219:GLN:N	2.43	0.49
1:B:2162:LEU:HA	1:B:2168:GLU:CB	2.42	0.49
1:A:412:LYS:HA	1:A:1257:LYS:CB	2.43	0.49
1:A:1090:ARG:O	1:A:1176:VAL:HA	2.12	0.49
1:A:1657:LYS:O	1:A:1660:LYS:N	2.44	0.49
1:B:769:SER:CB	1:B:779:ALA:HB2	2.43	0.49
1:B:1064:LEU:O	1:B:1068:THR:N	2.46	0.49
1:B:1284:CYS:C	1:B:1286:GLU:N	2.70	0.49
1:B:1810:LEU:O	1:B:1813:ASN:CB	2.60	0.49
1:B:1791:LEU:O	1:B:1795:GLN:CB	2.61	0.49
1:A:1253:ALA:HA	1:A:1256:HIS:CB	2.43	0.49
1:A:2056:THR:O	1:A:2059:SER:N	2.45	0.49
1:B:10:HIS:HA	1:B:114:VAL:HA	1.93	0.49
1:B:760:ASP:O	1:B:761:VAL:C	2.55	0.49
1:B:780:SER:O	1:B:781:PHE:C	2.53	0.49
1:B:997:PHE:O	1:B:998:LYS:C	2.56	0.49
1:B:2151:VAL:C	1:B:2154:ASN:H	2.21	0.49
1:A:388:VAL:N	1:A:430:PHE:O	2.46	0.49
1:A:398:TRP:O	1:A:399:VAL:C	2.55	0.49
1:A:606:LEU:O	1:A:607:GLU:C	2.56	0.49
1:A:772:ASN:O	1:A:773:LEU:C	2.55	0.49
1:A:1251:ASN:CB	1:A:1283:LEU:CA	2.90	0.49
1:A:1251:ASN:CB	1:A:1283:LEU:O	2.61	0.49
1:A:1973:GLN:O	1:A:1974:LEU:C	2.55	0.49
1:B:235:LYS:O	1:B:236:GLY:O	2.29	0.49
1:B:860:ASN:O	1:B:861:LYS:C	2.53	0.49
1:B:976:GLU:O	1:B:977:ILE:C	2.56	0.49
1:B:1130:GLU:HA	1:B:1133:VAL:O	2.12	0.49
1:A:833:PHE:O	1:A:836:THR:CA	2.61	0.49
1:A:2064:ILE:O	1:A:2065:ILE:C	2.55	0.49
1:B:104:GLU:O	1:B:105:THR:C	2.55	0.49
1:B:701:ARG:O	1:B:702:ASP:C	2.56	0.49
1:B:962:LYS:O	1:B:966:MET:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:970:THR:O	1:B:973:LYS:CB	2.61	0.49
1:B:1081:GLN:O	1:B:1082:LEU:C	2.56	0.49
1:B:1285:SER:C	1:B:1287:ILE:H	2.21	0.49
1:B:1677:THR:O	1:B:1680:GLU:N	2.39	0.49
1:B:2023:TYR:O	1:B:2025:ASN:N	2.46	0.49
1:A:1061:LEU:CB	1:A:1101:GLN:CB	2.91	0.49
1:B:688:GLU:O	1:B:691:GLU:N	2.46	0.49
1:B:695:GLU:O	1:B:696:VAL:O	2.31	0.49
1:A:519:ILE:O	1:A:520:PHE:C	2.56	0.48
1:A:966:MET:O	1:A:967:VAL:C	2.55	0.48
1:B:1115:ILE:C	1:B:1117:GLN:N	2.66	0.48
1:A:838:GLU:O	1:A:840:VAL:N	2.46	0.48
1:A:993:LEU:O	1:A:994:LEU:C	2.56	0.48
1:B:1884:LYS:CB	1:B:1886:LYS:H	2.27	0.48
1:A:1362:ARG:O	1:A:1363:ASP:C	2.56	0.48
1:B:1051:ASP:O	1:B:1055:HIS:CB	2.62	0.48
1:B:1432:ASP:C	1:B:1493:PRO:CB	2.86	0.48
1:B:1625:LEU:O	1:B:1628:VAL:CA	2.61	0.48
1:B:2088:LYS:O	1:B:2091:ALA:N	2.46	0.48
1:B:2182:ASP:O	1:B:2184:ALA:N	2.47	0.48
1:A:827:ASP:O	1:A:830:LYS:CB	2.61	0.48
1:B:224:MET:HA	1:B:293:ARG:CB	2.43	0.48
1:B:971:LYS:C	1:B:973:LYS:N	2.71	0.48
1:A:779:ALA:O	1:A:782:CYS:N	2.46	0.48
1:B:1460:ALA:O	1:B:1461:CYS:CB	2.62	0.48
1:A:1049:PRO:O	1:A:1050:LEU:C	2.55	0.48
1:B:1215:LEU:O	1:B:1219:GLN:CB	2.62	0.48
1:B:1480:GLU:CB	1:B:1883:ASN:CB	2.92	0.48
1:B:2014:THR:O	1:B:2067:ALA:CB	2.61	0.48
1:A:999:ARG:HA	1:A:1007:GLN:HA	1.94	0.48
1:A:2094:LEU:O	1:A:2095:LEU:C	2.55	0.48
1:B:597:ALA:O	1:B:598:LEU:C	2.55	0.48
1:B:679:GLY:O	1:B:680:VAL:C	2.55	0.48
1:B:763:LEU:O	1:B:767:CYS:CB	2.61	0.48
1:B:967:VAL:C	1:B:969:ASP:H	2.21	0.48
1:A:632:ASP:O	1:A:635:SER:N	2.46	0.48
1:A:680:VAL:C	1:A:682:THR:H	2.22	0.48
1:A:2064:ILE:O	1:A:2067:ALA:N	2.44	0.48
1:A:2185:LEU:O	1:A:2188:TYR:CB	2.61	0.48
1:B:307:HIS:O	1:B:308:LEU:C	2.57	0.48
1:B:1665:GLU:O	1:B:1666:ASN:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HA	1:A:207:ASN:O	2.14	0.48
1:A:1215:LEU:C	1:A:1217:LEU:N	2.71	0.48
1:A:1488:THR:O	1:A:1489:PHE:C	2.56	0.48
1:B:290:ASP:O	1:B:292:CYS:N	2.47	0.48
1:A:982:LEU:O	1:A:983:ASN:C	2.55	0.48
1:A:1800:LYS:O	1:A:1801:GLU:O	2.31	0.48
1:A:1861:ASP:O	1:A:1865:VAL:CB	2.62	0.48
1:B:685:ASN:O	1:B:686:ALA:C	2.53	0.48
1:B:831:GLU:O	1:B:832:ARG:C	2.56	0.48
1:B:855:SER:O	1:B:856:ASP:C	2.54	0.48
1:B:2111:ILE:O	1:B:2113:TYR:N	2.47	0.48
1:A:506:ARG:O	1:A:510:MET:HG2	2.14	0.47
1:A:975:ILE:O	1:A:979:GLN:CA	2.62	0.47
1:A:1201:GLN:O	1:A:1202:GLN:C	2.57	0.47
1:A:2167:LYS:O	1:A:2170:GLN:CB	2.62	0.47
1:B:870:ALA:HA	1:B:873:LEU:CB	2.44	0.47
1:A:560:LEU:O	1:A:561:ARG:C	2.57	0.47
1:A:834:ALA:O	1:A:835:GLN:C	2.55	0.47
1:A:973:LYS:O	1:A:977:ILE:CB	2.61	0.47
1:A:1197:SER:O	1:A:1198:ARG:C	2.57	0.47
1:A:1207:ASN:C	1:A:1209:GLY:N	2.72	0.47
1:A:2164:ARG:O	1:A:2165:HIS:CB	2.63	0.47
1:A:2184:ALA:HA	1:A:2187:PHE:CB	2.43	0.47
1:B:769:SER:CB	1:B:779:ALA:HA	2.43	0.47
1:B:1796:CYS:O	1:B:1797:HIS:C	2.56	0.47
1:B:1850:LYS:O	1:B:1854:LYS:N	2.47	0.47
1:A:438:ALA:O	1:A:439:GLU:C	2.55	0.47
1:A:761:VAL:O	1:A:764:ILE:CB	2.62	0.47
1:A:1449:LEU:O	1:A:1453:PHE:CB	2.62	0.47
1:A:1654:LYS:O	1:A:1655:LEU:C	2.57	0.47
1:B:573:TYR:O	1:B:577:GLN:N	2.47	0.47
1:B:694:GLU:O	1:B:696:VAL:N	2.48	0.47
1:B:864:PHE:O	1:B:865:GLU:C	2.51	0.47
1:B:885:LEU:O	1:B:888:THR:CB	2.62	0.47
1:B:1610:LEU:O	1:B:1614:LEU:CB	2.62	0.47
1:B:1986:PHE:C	1:B:1988:ARG:N	2.69	0.47
1:A:475:LYS:O	1:A:478:GLU:N	2.47	0.47
1:B:695:GLU:O	1:B:699:PHE:CB	2.61	0.47
1:B:830:LYS:O	1:B:831:GLU:C	2.56	0.47
1:B:1246:ALA:C	1:B:1248:ASN:N	2.71	0.47
1:A:1661:GLN:O	1:A:1663:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1864:LYS:O	1:A:1866:ALA:N	2.47	0.47
1:A:2058:GLU:O	1:A:2060:ASN:N	2.48	0.47
1:B:126:LEU:O	1:B:129:ASN:N	2.48	0.47
1:B:666:ILE:H	1:B:667:GLU:HA	1.79	0.47
1:B:2061:GLY:C	1:B:2064:ILE:H	2.18	0.47
1:B:2142:GLU:N	1:B:2143:ASP:CB	2.78	0.47
1:A:387:TYR:HA	1:A:431:ALA:HA	1.95	0.47
1:A:598:LEU:O	1:A:602:ASN:N	2.48	0.47
1:A:1083:LEU:O	1:A:1084:PHE:C	2.57	0.47
1:A:1251:ASN:O	1:A:1255:LEU:CB	2.62	0.47
1:A:2044:GLN:HA	1:A:2097:ALA:HB1	1.97	0.47
1:B:580:PHE:O	1:B:581:MET:C	2.56	0.47
1:B:1080:LEU:O	1:B:1084:PHE:N	2.39	0.47
1:B:1867:GLN:O	1:B:1871:LYS:CB	2.62	0.47
1:A:708:ARG:N	1:A:711:SER:H	2.13	0.47
1:A:845:ARG:O	1:A:848:VAL:CB	2.62	0.47
1:A:871:ARG:O	1:A:872:ASN:C	2.54	0.47
1:A:891:LEU:O	1:A:894:ILE:N	2.48	0.47
1:A:1631:ARG:O	1:A:1632:PRO:C	2.58	0.47
1:A:2026:GLU:O	1:A:2027:LYS:C	2.57	0.47
1:A:2177:GLY:O	1:A:2178:GLN:CB	2.62	0.47
1:A:2179:VAL:O	1:A:2180:ASP:C	2.58	0.47
1:B:969:ASP:O	1:B:971:LYS:N	2.48	0.47
1:B:976:GLU:C	1:B:978:LEU:H	2.23	0.47
1:B:1350:SER:O	1:B:1351:PHE:C	2.57	0.47
1:B:1461:CYS:O	1:B:1462:ASN:CB	2.63	0.47
1:B:1821:HIS:O	1:B:1825:LEU:CB	2.63	0.47
1:A:2180:ASP:O	1:A:2184:ALA:N	2.48	0.47
1:B:729:ILE:O	1:B:730:LEU:C	2.56	0.47
1:B:890:ILE:O	1:B:893:ALA:HB3	2.14	0.47
1:B:1238:HIS:CB	1:B:1282:GLN:CB	2.93	0.47
1:A:10:HIS:CB	1:A:112:GLY:O	2.63	0.47
1:A:666:ILE:CB	1:A:669:LYS:C	2.88	0.47
1:A:1998:LEU:O	1:A:1999:VAL:C	2.55	0.47
1:A:2061:GLY:O	1:A:2062:ILE:C	2.58	0.47
1:B:103:ASN:O	1:B:104:GLU:C	2.58	0.47
1:B:642:ASN:O	1:B:643:LYS:C	2.58	0.47
1:B:1086:HIS:C	1:B:1088:SER:H	2.22	0.47
1:B:2026:GLU:O	1:B:2027:LYS:C	2.57	0.47
1:A:708:ARG:C	1:A:712:VAL:H	2.13	0.47
1:A:1803:ALA:HB1	1:A:1842:PHE:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:MET:O	1:B:642:ASN:C	2.58	0.47
1:B:769:SER:O	1:B:772:ASN:C	2.58	0.47
1:B:1445:HIS:O	1:B:1446:MET:CB	2.63	0.47
1:B:1872:ALA:C	1:B:1874:VAL:H	2.23	0.47
1:B:2032:ILE:O	1:B:2035:THR:N	2.48	0.47
1:A:610:ILE:O	1:A:613:ALA:HB3	2.15	0.46
1:A:827:ASP:O	1:A:830:LYS:N	2.49	0.46
1:A:1849:ASP:O	1:A:1850:LYS:C	2.58	0.46
1:B:1312:LEU:O	1:B:1313:GLN:C	2.57	0.46
1:B:1986:PHE:O	1:B:1988:ARG:CA	2.62	0.46
1:A:992:CYS:C	1:A:994:LEU:N	2.72	0.46
1:A:1420:ILE:C	1:A:1424:ASN:H	2.22	0.46
1:A:2043:CYS:C	1:A:2097:ALA:HB1	2.40	0.46
1:B:48:ASN:O	1:B:49:PRO:C	2.58	0.46
1:B:549:PHE:O	1:B:552:ILE:N	2.48	0.46
1:B:645:ILE:O	1:B:646:PRO:C	2.56	0.46
1:B:708:ARG:O	1:B:709:SER:C	2.59	0.46
1:B:836:THR:O	1:B:839:PHE:N	2.48	0.46
1:B:1795:GLN:O	1:B:1799:ASP:N	2.48	0.46
1:A:749:TYR:C	1:A:751:ALA:N	2.71	0.46
1:A:1245:CYS:CB	1:A:1341:VAL:H	2.26	0.46
1:A:1463:ASN:O	1:A:1464:THR:CB	2.62	0.46
1:A:1605:ASP:O	1:A:1609:ALA:CB	2.64	0.46
1:A:1864:LYS:O	1:A:1866:ALA:C	2.53	0.46
1:B:732:TYR:O	1:B:733:TYR:C	2.58	0.46
1:B:1118:ASP:O	1:B:1119:LEU:C	2.56	0.46
1:B:1459:ARG:C	1:B:1461:CYS:N	2.73	0.46
1:B:1634:LEU:O	1:B:1638:GLU:O	2.33	0.46
1:A:842:GLU:O	1:A:843:TYR:C	2.59	0.46
1:A:1070:HIS:O	1:A:1071:ASP:C	2.59	0.46
1:B:856:ASP:O	1:B:860:ASN:CB	2.64	0.46
1:B:960:PRO:N	1:B:961:GLU:HA	2.30	0.46
1:B:2153:HIS:HA	1:B:2156:TYR:CB	2.45	0.46
1:A:230:LYS:HA	1:A:232:ASP:N	2.30	0.46
1:A:868:ASN:O	1:A:869:LEU:C	2.56	0.46
1:A:1214:VAL:O	1:A:1218:LEU:CB	2.64	0.46
1:B:173:GLY:O	1:B:174:ASP:C	2.58	0.46
1:B:980:PHE:O	1:B:981:ILE:C	2.59	0.46
1:B:1293:GLN:CA	1:B:1345:TYR:HA	2.46	0.46
1:A:768:MET:O	1:A:769:SER:C	2.59	0.46
1:A:772:ASN:C	1:A:774:PRO:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:VAL:C	1:A:900:VAL:CA	2.85	0.46
1:A:1223:GLU:CB	1:A:1228:THR:CB	2.93	0.46
1:A:1461:CYS:CB	1:A:1465:SER:CB	2.93	0.46
1:A:1843:PHE:O	1:A:1844:CYS:C	2.58	0.46
1:A:2032:ILE:O	1:A:2033:ASN:C	2.58	0.46
1:B:686:ALA:O	1:B:689:ALA:HB3	2.15	0.46
1:B:885:LEU:O	1:B:888:THR:CA	2.63	0.46
1:A:617:THR:O	1:A:621:LEU:N	2.32	0.46
1:A:689:ALA:O	1:A:690:GLY:C	2.59	0.46
1:A:1062:ARG:O	1:A:1063:VAL:C	2.59	0.46
1:A:1251:ASN:O	1:A:1255:LEU:N	2.45	0.46
1:A:2006:LEU:O	1:A:2007:ASP:C	2.58	0.46
1:B:1231:GLN:CA	1:B:1275:HIS:CB	2.93	0.46
1:B:1459:ARG:O	1:B:1461:CYS:N	2.49	0.46
1:B:1624:VAL:O	1:B:1627:ASP:CB	2.64	0.46
1:A:480:LEU:O	1:A:482:TYR:N	2.49	0.46
1:A:631:LEU:O	1:A:634:LEU:CB	2.64	0.46
1:A:2055:ALA:O	1:A:2059:SER:CA	2.64	0.46
1:A:2174:LYS:O	1:A:2177:GLY:O	2.33	0.46
1:B:888:THR:C	1:B:891:LEU:H	2.24	0.46
1:B:992:CYS:O	1:B:994:LEU:N	2.48	0.46
1:B:1072:TYR:N	1:B:1106:SER:CB	2.79	0.46
1:A:277:SER:O	1:A:280:ALA:N	2.48	0.46
1:A:446:ALA:O	1:A:447:ASN:C	2.57	0.46
1:A:724:LYS:O	1:A:726:ASP:N	2.45	0.46
1:B:856:ASP:O	1:B:857:LYS:C	2.57	0.46
1:B:1059:THR:O	1:B:1060:PHE:C	2.56	0.46
1:B:1086:HIS:C	1:B:1088:SER:N	2.74	0.46
1:B:1200:GLN:O	1:B:1203:ARG:N	2.49	0.46
1:B:1228:THR:CA	1:B:1271:VAL:CB	2.92	0.46
1:B:1988:ARG:C	1:B:1990:GLN:H	2.23	0.46
1:A:571:GLN:C	1:A:573:TYR:N	2.74	0.46
1:A:883:ASP:O	1:A:884:LEU:C	2.57	0.46
1:A:1100:VAL:O	1:A:1101:GLN:C	2.57	0.46
1:A:1223:GLU:O	1:A:1271:VAL:CB	2.63	0.46
1:B:1191:SER:O	1:B:1239:GLU:CB	2.63	0.46
1:B:1845:ARG:O	1:B:1848:GLU:N	2.49	0.46
1:A:2173:LEU:O	1:A:2177:GLY:N	2.49	0.45
1:A:554:ARG:CB	1:A:557:TYR:CB	2.94	0.45
1:A:833:PHE:O	1:A:834:ALA:C	2.60	0.45
1:A:867:VAL:O	1:A:868:ASN:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:ILE:O	1:A:982:LEU:C	2.59	0.45
1:B:110:LEU:O	1:B:113:THR:CB	2.64	0.45
1:B:549:PHE:C	1:B:551:HIS:H	2.24	0.45
1:B:752:ILE:O	1:B:753:ASN:C	2.59	0.45
1:B:857:LYS:O	1:B:858:GLU:O	2.34	0.45
1:A:276:THR:O	1:A:508:LYS:NZ	2.38	0.45
1:A:653:CYS:O	1:A:657:LEU:N	2.48	0.45
1:B:52:LYS:C	1:B:54:ARG:H	2.24	0.45
1:B:666:ILE:CB	1:B:669:LYS:N	2.79	0.45
1:B:1798:LEU:CA	1:B:1802:GLY:H	2.29	0.45
1:A:894:ILE:O	1:A:898:VAL:N	2.50	0.45
1:A:1285:SER:C	1:A:1341:VAL:CB	2.89	0.45
1:B:560:LEU:C	1:B:562:HIS:N	2.73	0.45
1:B:754:GLU:O	1:B:758:GLN:N	2.43	0.45
1:B:1679:ARG:O	1:B:1687:GLY:C	2.60	0.45
1:A:257:ARG:C	1:A:259:LYS:N	2.74	0.45
1:A:411:GLU:O	1:A:412:LYS:CB	2.64	0.45
1:A:439:GLU:O	1:A:440:VAL:C	2.59	0.45
1:A:649:GLN:O	1:A:652:ILE:CB	2.64	0.45
1:A:1194:VAL:O	1:A:1197:SER:CA	2.63	0.45
1:A:1207:ASN:C	1:A:1209:GLY:H	2.24	0.45
1:A:1303:GLY:O	1:A:1304:ARG:C	2.59	0.45
1:B:1433:THR:HA	1:B:1493:PRO:N	2.32	0.45
1:B:2117:PRO:HA	1:B:2171:THR:CB	2.46	0.45
1:A:1634:LEU:C	1:A:1646:CYS:CB	2.89	0.45
1:B:263:PHE:CB	1:B:416:LEU:O	2.65	0.45
1:B:988:TYR:O	1:B:989:ARG:C	2.56	0.45
1:B:1224:LYS:O	1:B:1227:ASP:O	2.35	0.45
1:B:1682:MET:O	1:B:1683:THR:C	2.57	0.45
1:B:1850:LYS:C	1:B:1854:LYS:CB	2.90	0.45
1:A:832:ARG:O	1:A:833:PHE:C	2.59	0.45
1:A:888:THR:O	1:A:889:LYS:C	2.60	0.45
1:A:1270:ALA:HB2	1:A:1319:GLU:CB	2.46	0.45
1:B:271:SER:O	1:B:273:THR:N	2.50	0.45
1:B:712:VAL:O	1:B:713:ARG:C	2.59	0.45
1:B:1194:VAL:C	1:B:1197:SER:H	2.25	0.45
1:B:1284:CYS:O	1:B:1285:SER:C	2.59	0.45
1:B:2169:LEU:O	1:B:2170:GLN:C	2.58	0.45
1:A:93:HIS:O	1:A:94:HIS:C	2.60	0.45
1:B:110:LEU:O	1:B:111:LEU:C	2.58	0.45
1:B:855:SER:C	1:B:857:LYS:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1059:THR:C	1:B:1061:LEU:N	2.73	0.45
1:B:1223:GLU:O	1:B:1270:ALA:O	2.34	0.45
1:B:1238:HIS:O	1:B:1239:GLU:C	2.60	0.45
1:B:1246:ALA:C	1:B:1248:ASN:H	2.24	0.45
1:B:1272:THR:O	1:B:1275:HIS:N	2.49	0.45
1:B:1634:LEU:O	1:B:1638:GLU:C	2.60	0.45
1:B:1854:LYS:O	1:B:1857:LYS:CB	2.65	0.45
1:A:12:GLY:C	1:A:226:TRP:CB	2.90	0.45
1:A:665:LEU:O	1:A:670:LEU:C	2.59	0.45
1:A:840:VAL:O	1:A:841:GLU:C	2.59	0.45
1:A:2062:ILE:O	1:A:2065:ILE:N	2.50	0.45
1:B:1842:PHE:O	1:B:1843:PHE:C	2.60	0.45
1:A:970:THR:C	1:A:973:LYS:CB	2.90	0.45
1:A:1084:PHE:O	1:A:1085:ARG:C	2.60	0.45
1:B:654:LYS:O	1:B:658:ASN:N	2.31	0.45
1:B:865:GLU:O	1:B:869:LEU:CB	2.65	0.45
1:B:1405:ILE:O	1:B:1406:VAL:C	2.60	0.45
1:A:447:ASN:O	1:A:448:ASP:C	2.59	0.44
1:A:1108:ASP:O	1:A:1109:VAL:C	2.59	0.44
1:B:314:LEU:O	1:B:366:SER:HA	2.17	0.44
1:B:588:ASP:CB	1:B:591:ALA:HB3	2.47	0.44
1:B:611:THR:C	1:B:613:ALA:H	2.25	0.44
1:B:622:VAL:O	1:B:625:ASN:O	2.34	0.44
1:B:969:ASP:C	1:B:971:LYS:N	2.71	0.44
1:B:1287:ILE:CB	1:B:1341:VAL:CB	2.95	0.44
1:B:1632:PRO:C	1:B:1634:LEU:N	2.74	0.44
1:B:2060:ASN:O	1:B:2061:GLY:C	2.59	0.44
1:B:2087:LEU:O	1:B:2091:ALA:HB3	2.16	0.44
1:A:103:ASN:O	1:A:104:GLU:C	2.61	0.44
1:A:969:ASP:C	1:A:971:LYS:N	2.71	0.44
1:A:1037:ALA:C	1:A:1039:GLY:N	2.73	0.44
1:B:131:TYR:O	1:B:151:LEU:HA	2.17	0.44
1:B:504:ARG:HA	1:B:507:GLN:OE1	2.18	0.44
1:B:611:THR:O	1:B:612:ALA:C	2.60	0.44
1:B:611:THR:O	1:B:613:ALA:N	2.50	0.44
1:B:829:ILE:O	1:B:832:ARG:CB	2.65	0.44
1:B:1218:LEU:C	1:B:1220:ILE:H	2.24	0.44
1:B:1859:PHE:O	1:B:1860:TYR:C	2.61	0.44
1:B:2005:PHE:O	1:B:2008:CYS:N	2.50	0.44
1:B:2153:HIS:O	1:B:2157:ILE:CB	2.65	0.44
1:A:858:GLU:O	1:A:859:LYS:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:THR:C	1:A:1050:LEU:N	2.75	0.44
1:A:1679:ARG:O	1:A:1682:MET:N	2.51	0.44
1:B:780:SER:O	1:B:783:ARG:CA	2.65	0.44
1:B:1233:ILE:O	1:B:1234:MET:C	2.60	0.44
1:B:1630:HIS:O	1:B:1633:GLU:N	2.50	0.44
1:B:1824:ILE:O	1:B:1825:LEU:C	2.60	0.44
1:B:2061:GLY:O	1:B:2064:ILE:CA	2.64	0.44
1:A:520:PHE:O	1:A:522:LEU:N	2.51	0.44
1:A:549:PHE:O	1:A:551:HIS:N	2.51	0.44
1:A:779:ALA:O	1:A:780:SER:C	2.60	0.44
1:A:2116:ARG:O	1:A:2117:PRO:C	2.59	0.44
1:A:2120:LEU:O	1:A:2124:ILE:CB	2.65	0.44
1:A:2203:THR:O	1:A:2204:MET:CB	2.65	0.44
1:B:2127:ALA:O	1:B:2128:TYR:C	2.59	0.44
1:A:1194:VAL:C	1:A:1197:SER:H	2.26	0.44
1:A:1488:THR:O	1:A:1490:PHE:N	2.50	0.44
1:A:1677:THR:O	1:A:1680:GLU:N	2.50	0.44
1:A:1847:THR:O	1:A:1850:LYS:N	2.49	0.44
1:A:749:TYR:O	1:A:750:LEU:C	2.61	0.44
1:A:764:ILE:O	1:A:765:LEU:C	2.60	0.44
1:A:1371:LEU:CB	1:A:1374:HIS:C	2.91	0.44
1:A:1371:LEU:CB	1:A:1374:HIS:CB	2.95	0.44
1:A:1975:LEU:O	1:A:1976:CYS:C	2.59	0.44
1:B:568:ARG:HH11	1:B:572:GLU:CD	2.26	0.44
1:B:981:ILE:O	1:B:982:LEU:O	2.35	0.44
1:B:1080:LEU:O	1:B:1081:GLN:C	2.61	0.44
1:A:478:GLU:O	1:A:479:ASP:C	2.59	0.44
1:A:1001:PHE:O	1:A:1003:GLU:N	2.48	0.44
1:A:1434:GLU:O	1:A:1492:SER:CB	2.65	0.44
1:A:2005:PHE:O	1:A:2006:LEU:C	2.57	0.44
1:B:591:ALA:O	1:B:592:GLU:C	2.59	0.44
1:B:967:VAL:O	1:B:968:MET:C	2.60	0.44
1:B:986:LEU:O	1:B:987:ASP:C	2.60	0.44
1:B:1213:VAL:O	1:B:1214:VAL:O	2.35	0.44
1:A:101:LYS:O	1:A:102:GLN:C	2.58	0.44
1:A:1215:LEU:O	1:A:1216:GLU:C	2.61	0.44
1:A:1841:SER:O	1:A:1842:PHE:C	2.61	0.44
1:A:1856:PHE:O	1:A:1857:LYS:C	2.61	0.44
1:A:2201:ASP:O	1:A:2202:ARG:CB	2.66	0.44
1:B:1656:ILE:O	1:B:1657:LYS:C	2.59	0.44
1:B:1974:LEU:O	1:B:1975:LEU:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:LEU:O	1:A:845:ARG:C	2.57	0.44
1:A:870:ALA:O	1:A:871:ARG:C	2.56	0.44
1:A:972:LEU:C	1:A:974:ILE:N	2.76	0.44
1:A:1116:LYS:O	1:A:1119:LEU:CB	2.66	0.44
1:A:1117:GLN:C	1:A:1119:LEU:H	2.26	0.44
1:A:1654:LYS:O	1:A:1657:LYS:N	2.51	0.44
1:A:1792:ALA:CB	1:B:1792:ALA:CB	2.96	0.44
1:A:1884:LYS:O	1:A:1885:LYS:C	2.61	0.44
1:A:1953:LYS:O	1:A:1954:ASP:C	2.57	0.44
1:A:2103:HIS:O	1:A:2104:ASP:CB	2.66	0.44
1:B:745:LEU:O	1:B:1075:LEU:CB	2.66	0.44
1:A:1855:PHE:C	1:A:1857:LYS:N	2.74	0.43
1:A:1857:LYS:C	1:A:1859:PHE:N	2.70	0.43
1:A:1968:ILE:O	1:A:1969:LEU:C	2.60	0.43
1:A:2088:LYS:O	1:A:2092:SER:CB	2.66	0.43
1:B:769:SER:O	1:B:772:ASN:O	2.36	0.43
1:B:1071:ASP:C	1:B:1106:SER:CB	2.91	0.43
1:B:2061:GLY:C	1:B:2063:ASP:N	2.75	0.43
1:A:613:ALA:O	1:A:614:GLU:C	2.56	0.43
1:A:1097:PHE:O	1:A:1098:LYS:C	2.59	0.43
1:A:1378:VAL:O	1:A:1382:ALA:CB	2.65	0.43
1:A:1417:GLU:C	1:A:1419:LYS:N	2.74	0.43
1:A:1661:GLN:C	1:A:1663:LEU:N	2.74	0.43
1:B:91:LYS:O	1:B:94:HIS:N	2.51	0.43
1:B:1102:LEU:O	1:B:1103:LEU:C	2.59	0.43
1:B:1484:SER:N	1:B:1884:LYS:O	2.51	0.43
1:B:1682:MET:O	1:B:1686:ARG:CA	2.63	0.43
1:B:2087:LEU:O	1:B:2091:ALA:HB2	2.17	0.43
1:B:2118:LYS:O	1:B:2119:GLU:C	2.60	0.43
1:A:885:LEU:O	1:A:886:ARG:C	2.61	0.43
1:A:1375:ILE:HA	1:A:1378:VAL:H	1.84	0.43
1:A:1417:GLU:O	1:A:1420:ILE:N	2.52	0.43
1:A:1653:CYS:O	1:A:1656:ILE:CB	2.66	0.43
1:A:1870:ILE:O	1:A:1871:LYS:C	2.61	0.43
1:A:1991:ASN:O	1:A:1992:ASN:C	2.61	0.43
1:A:2020:LEU:O	1:A:2024:ILE:CB	2.66	0.43
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.51	0.43
1:B:690:GLY:O	1:B:691:GLU:C	2.61	0.43
1:B:768:MET:O	1:B:769:SER:C	2.60	0.43
1:B:1213:VAL:C	1:B:1214:VAL:O	2.62	0.43
1:B:1285:SER:O	1:B:1287:ILE:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ALA:HB1	1:A:95:ALA:HB1	2.00	0.43
1:A:473:VAL:O	1:A:474:THR:C	2.61	0.43
1:A:696:VAL:O	1:A:697:TRP:C	2.60	0.43
1:A:765:LEU:O	1:A:766:ARG:C	2.62	0.43
1:B:756:SER:O	1:B:757:GLY:C	2.59	0.43
1:B:1286:GLU:CB	1:B:1289:GLU:CB	2.96	0.43
1:B:1488:THR:O	1:B:1492:SER:C	2.61	0.43
1:B:1797:HIS:C	1:B:1802:GLY:HA3	2.43	0.43
1:A:1841:SER:O	1:A:1842:PHE:O	2.36	0.43
1:A:1966:GLN:HA	1:A:1969:LEU:CB	2.48	0.43
1:B:605:LEU:O	1:B:606:LEU:C	2.60	0.43
1:B:693:GLU:O	1:B:697:TRP:CB	2.67	0.43
1:B:1376:HIS:C	1:B:1378:VAL:N	2.77	0.43
1:A:553:CYS:C	1:A:555:LEU:N	2.77	0.43
1:A:838:GLU:C	1:A:840:VAL:N	2.75	0.43
1:A:989:ARG:O	1:A:990:ILE:CB	2.67	0.43
1:B:560:LEU:O	1:B:562:HIS:N	2.52	0.43
1:B:1828:ILE:O	1:B:1829:ALA:C	2.62	0.43
1:B:1963:THR:HA	1:B:1966:GLN:CB	2.48	0.43
1:A:267:THR:OG1	1:A:275:ALA:HB2	2.18	0.43
1:A:1007:GLN:C	1:A:1009:SER:N	2.75	0.43
1:A:1316:VAL:C	1:A:1319:GLU:H	2.26	0.43
1:A:1477:TYR:CB	1:A:1881:LEU:CB	2.96	0.43
1:B:504:ARG:O	1:B:507:GLN:N	2.51	0.43
1:B:621:LEU:O	1:B:625:ASN:CA	2.65	0.43
1:B:689:ALA:O	1:B:690:GLY:C	2.61	0.43
1:B:781:PHE:O	1:B:782:CYS:C	2.60	0.43
1:B:1328:ASP:C	1:B:1330:VAL:N	2.76	0.43
1:B:1839:GLN:O	1:B:1842:PHE:CB	2.67	0.43
1:B:2120:LEU:O	1:B:2121:VAL:C	2.61	0.43
1:A:99:GLU:O	1:A:100:LYS:C	2.60	0.43
1:A:199:GLN:HA	1:A:206:CYS:O	2.18	0.43
1:A:479:ASP:O	1:A:482:TYR:CB	2.67	0.43
1:A:516:LEU:O	1:A:517:LYS:C	2.61	0.43
1:A:619:VAL:O	1:A:620:SER:C	2.60	0.43
1:A:1295:PHE:O	1:A:1297:HIS:N	2.51	0.43
1:A:1341:VAL:O	1:A:1344:PHE:N	2.52	0.43
1:B:786:LEU:O	1:B:790:VAL:N	2.44	0.43
1:B:853:PRO:O	1:B:855:SER:N	2.51	0.43
1:B:1629:LEU:O	1:B:1632:PRO:CB	2.66	0.43
1:B:1661:GLN:O	1:B:1662:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:CB	1:A:110:LEU:O	2.66	0.43
1:A:597:ALA:O	1:A:598:LEU:C	2.61	0.43
1:A:842:GLU:C	1:A:844:LEU:N	2.74	0.43
1:A:1952:ALA:O	1:A:1954:ASP:N	2.52	0.43
1:A:2123:VAL:O	1:A:2127:ALA:CB	2.67	0.43
1:B:32:LEU:CB	1:B:445:PHE:HA	2.49	0.43
1:B:568:ARG:NH1	1:B:572:GLU:CD	2.77	0.43
1:B:619:VAL:O	1:B:620:SER:C	2.62	0.43
1:B:769:SER:O	1:B:773:LEU:CA	2.66	0.43
1:B:1251:ASN:O	1:B:1252:GLN:C	2.60	0.43
1:B:1991:ASN:O	1:B:1992:ASN:O	2.36	0.43
1:B:2003:LEU:O	1:B:2004:GLN:C	2.58	0.43
1:B:2044:GLN:O	1:B:2046:PRO:N	2.51	0.43
1:A:567:TYR:O	1:A:571:GLN:HG3	2.18	0.43
1:A:684:GLU:O	1:A:685:ASN:C	2.61	0.43
1:A:1973:GLN:C	1:A:1975:LEU:N	2.71	0.43
1:B:696:VAL:O	1:B:698:LEU:N	2.52	0.43
1:B:766:ARG:O	1:B:767:CYS:C	2.61	0.43
1:B:863:THR:O	1:B:867:VAL:CB	2.67	0.43
1:B:1622:LEU:O	1:B:1623:SER:C	2.62	0.43
1:B:2061:GLY:O	1:B:2063:ASP:N	2.52	0.43
1:B:2193:ALA:C	1:B:2195:ILE:N	2.76	0.43
1:A:12:GLY:O	1:A:226:TRP:HA	2.19	0.42
1:A:841:GLU:O	1:A:844:LEU:CB	2.67	0.42
1:A:965:ILE:O	1:A:968:MET:CB	2.67	0.42
1:A:984:VAL:O	1:A:988:TYR:CB	2.67	0.42
1:A:1082:LEU:O	1:A:1083:LEU:C	2.61	0.42
1:A:1623:SER:O	1:A:1626:VAL:CB	2.67	0.42
1:A:1855:PHE:C	1:A:1857:LYS:H	2.26	0.42
1:A:2192:THR:O	1:A:2216:GLU:O	2.37	0.42
1:B:833:PHE:O	1:B:836:THR:CB	2.66	0.42
1:B:896:ASP:O	1:B:899:HIS:N	2.52	0.42
1:B:1082:LEU:O	1:B:1083:LEU:C	2.62	0.42
1:B:1432:ASP:O	1:B:1493:PRO:O	2.36	0.42
1:B:2164:ARG:O	1:B:2165:HIS:CB	2.67	0.42
1:A:480:LEU:O	1:A:483:PHE:N	2.53	0.42
1:A:899:HIS:N	1:A:900:VAL:CA	2.81	0.42
1:A:1471:ASP:O	1:A:1472:SER:C	2.61	0.42
1:A:1487:THR:O	1:A:1488:THR:C	2.60	0.42
1:A:1800:LYS:O	1:A:1801:GLU:C	2.62	0.42
1:A:1969:LEU:O	1:A:1970:ARG:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2192:THR:O	1:A:2216:GLU:CB	2.67	0.42
1:B:650:GLU:O	1:B:651:LEU:C	2.59	0.42
1:B:769:SER:CB	1:B:779:ALA:CA	2.97	0.42
1:B:1315:ILE:O	1:B:1318:ALA:N	2.51	0.42
1:B:1635:LEU:CA	1:B:1646:CYS:CB	2.96	0.42
1:B:1976:CYS:O	1:B:1977:GLU:C	2.59	0.42
1:B:2029:VAL:O	1:B:2030:ALA:C	2.61	0.42
1:B:2034:GLN:O	1:B:2035:THR:C	2.60	0.42
1:B:2182:ASP:C	1:B:2184:ALA:H	2.26	0.42
1:A:38:VAL:CA	1:A:207:ASN:O	2.67	0.42
1:A:689:ALA:O	1:A:691:GLU:N	2.52	0.42
1:A:729:ILE:O	1:A:732:TYR:CB	2.67	0.42
1:A:1436:GLU:CB	1:A:1493:PRO:C	2.92	0.42
1:A:2026:GLU:O	1:A:2028:ASN:N	2.51	0.42
1:A:2058:GLU:C	1:A:2060:ASN:N	2.76	0.42
1:B:10:HIS:CB	1:B:112:GLY:O	2.68	0.42
1:B:575:ALA:O	1:B:578:PHE:CB	2.67	0.42
1:B:687:LEU:O	1:B:688:GLU:C	2.62	0.42
1:B:730:LEU:O	1:B:731:SER:C	2.62	0.42
1:B:753:ASN:O	1:B:757:GLY:N	2.42	0.42
1:B:1062:ARG:O	1:B:1063:VAL:C	2.62	0.42
1:B:1291:VAL:O	1:B:1292:VAL:C	2.62	0.42
1:B:1417:GLU:O	1:B:1418:VAL:C	2.62	0.42
1:B:1620:ALA:O	1:B:1621:GLU:C	2.59	0.42
1:A:857:LYS:O	1:A:858:GLU:C	2.62	0.42
1:A:888:THR:O	1:A:891:LEU:CA	2.68	0.42
1:A:1273:MET:O	1:A:1274:GLN:C	2.63	0.42
1:A:1294:HIS:O	1:A:1298:CYS:CA	2.67	0.42
1:A:1640:THR:CB	1:A:1644:ARG:CB	2.97	0.42
1:B:613:ALA:O	1:B:614:GLU:C	2.61	0.42
1:B:1026:GLY:CA	1:B:1594:ARG:CB	2.98	0.42
1:B:1211:HIS:O	1:B:1214:VAL:CA	2.65	0.42
1:B:1240:PHE:CB	1:B:1245:CYS:HA	2.49	0.42
1:B:1383:VAL:O	1:B:1386:GLU:N	2.52	0.42
1:B:1480:GLU:C	1:B:1883:ASN:CB	2.92	0.42
1:B:1593:SER:O	1:B:1597:ARG:N	2.42	0.42
1:A:842:GLU:O	1:A:844:LEU:N	2.52	0.42
1:A:846:ASP:O	1:A:849:CYS:N	2.52	0.42
1:A:987:ASP:O	1:A:988:TYR:C	2.62	0.42
1:A:1112:TYR:HA	1:A:1115:ILE:CB	2.50	0.42
1:A:1634:LEU:CB	1:A:1646:CYS:CA	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1084:PHE:O	1:B:1085:ARG:C	2.60	0.42
1:B:1661:GLN:C	1:B:1663:LEU:N	2.76	0.42
1:B:2197:ILE:HA	1:B:2212:PRO:N	2.35	0.42
1:A:1474:LEU:C	1:A:1476:LYS:N	2.76	0.42
1:A:2030:ALA:O	1:A:2031:LEU:C	2.62	0.42
1:A:2150:ASN:O	1:A:2153:HIS:CA	2.65	0.42
1:B:315:ALA:HB2	1:B:366:SER:HA	2.01	0.42
1:B:438:ALA:O	1:B:439:GLU:C	2.60	0.42
1:B:684:GLU:O	1:B:687:LEU:CA	2.67	0.42
1:B:700:TRP:O	1:B:701:ARG:C	2.62	0.42
1:B:829:ILE:O	1:B:830:LYS:C	2.63	0.42
1:A:610:ILE:O	1:A:611:THR:C	2.59	0.42
1:B:560:LEU:O	1:B:561:ARG:C	2.61	0.42
1:B:869:LEU:O	1:B:871:ARG:N	2.53	0.42
1:B:1097:PHE:O	1:B:1098:LYS:C	2.63	0.42
1:B:1128:LYS:O	1:B:1132:TRP:CB	2.67	0.42
1:B:1248:ASN:C	1:B:1250:GLN:N	2.75	0.42
1:B:1990:GLN:O	1:B:1991:ASN:C	2.62	0.42
1:B:2036:LEU:O	1:B:2040:THR:CB	2.68	0.42
1:A:101:LYS:C	1:A:103:ASN:N	2.77	0.42
1:A:610:ILE:O	1:A:613:ALA:CB	2.67	0.42
1:B:606:LEU:O	1:B:607:GLU:C	2.59	0.42
1:B:2151:VAL:HA	1:B:2154:ASN:CB	2.50	0.42
1:A:10:HIS:HA	1:A:113:THR:O	2.19	0.42
1:A:593:ASP:O	1:A:594:THR:C	2.61	0.42
1:A:701:ARG:O	1:A:702:ASP:C	2.63	0.42
1:A:2200:LEU:CB	1:A:2209:PHE:O	2.67	0.42
1:B:1483:MET:HA	1:B:1486:VAL:CB	2.50	0.42
1:B:1655:LEU:O	1:B:1656:ILE:C	2.62	0.42
1:A:15:CYS:HA	1:A:223:PHE:H	1.84	0.42
1:A:518:GLN:O	1:A:519:ILE:C	2.58	0.42
1:A:972:LEU:O	1:A:974:ILE:N	2.52	0.42
1:B:640:SER:O	1:B:641:MET:C	2.63	0.42
1:B:834:ALA:O	1:B:835:GLN:C	2.61	0.42
1:B:862:LEU:O	1:B:866:VAL:N	2.48	0.42
1:B:980:PHE:C	1:B:982:LEU:N	2.77	0.42
1:B:990:ILE:O	1:B:991:SER:C	2.63	0.42
1:B:1854:LYS:C	1:B:1857:LYS:H	2.28	0.42
1:B:2032:ILE:O	1:B:2035:THR:CB	2.68	0.42
1:A:549:PHE:O	1:A:552:ILE:N	2.40	0.41
1:A:1042:GLY:O	1:A:1043:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1821:HIS:HA	1:A:1824:ILE:CB	2.50	0.41
1:B:91:LYS:O	1:B:92:LEU:C	2.62	0.41
1:B:181:LYS:HA	1:B:218:TRP:O	2.20	0.41
1:B:710:LYS:O	1:B:711:SER:C	2.62	0.41
1:B:742:ARG:CB	1:B:1040:ILE:CA	2.98	0.41
1:B:1619:GLN:O	1:B:1622:LEU:CB	2.68	0.41
1:A:436:SER:O	1:A:437:PRO:C	2.59	0.41
1:A:1338:GLY:O	1:A:1342:LEU:CB	2.68	0.41
1:A:1363:ASP:O	1:A:1366:ASP:CB	2.68	0.41
1:A:1851:LYS:C	1:A:1853:GLU:N	2.76	0.41
1:B:582:GLN:O	1:B:583:LYS:C	2.61	0.41
1:B:669:LYS:O	1:B:672:LEU:CB	2.68	0.41
1:B:742:ARG:CB	1:B:1040:ILE:HA	2.50	0.41
1:B:882:SER:O	1:B:886:ARG:N	2.46	0.41
1:B:990:ILE:O	1:B:993:LEU:N	2.53	0.41
1:B:1079:ALA:O	1:B:1080:LEU:C	2.63	0.41
1:B:1355:ILE:O	1:B:1356:GLN:CB	2.68	0.41
1:B:1805:ASN:O	1:B:1806:LEU:C	2.62	0.41
1:A:277:SER:C	1:A:279:LYS:N	2.78	0.41
1:A:606:LEU:O	1:A:608:LYS:N	2.53	0.41
1:A:701:ARG:O	1:A:703:SER:O	2.38	0.41
1:A:1379:GLU:HA	1:A:1382:ALA:CB	2.40	0.41
1:A:1793:GLU:HA	1:A:1796:CYS:CB	2.50	0.41
1:A:2044:GLN:C	1:A:2046:PRO:N	2.78	0.41
1:B:111:LEU:O	1:B:113:THR:N	2.53	0.41
1:B:271:SER:O	1:B:272:ALA:C	2.63	0.41
1:B:1858:VAL:O	1:B:1859:PHE:C	2.62	0.41
1:A:1040:ILE:O	1:A:1043:GLY:N	2.52	0.41
1:A:1477:TYR:HA	1:A:1881:LEU:O	2.20	0.41
1:A:1670:LEU:O	1:A:1671:CYS:C	2.60	0.41
1:B:439:GLU:O	1:B:442:ASP:N	2.53	0.41
1:B:751:ALA:O	1:B:752:ILE:C	2.63	0.41
1:B:1278:MET:O	1:B:1279:ASN:C	2.63	0.41
1:A:179:GLY:O	1:A:180:ASP:C	2.63	0.41
1:A:690:GLY:O	1:A:691:GLU:C	2.63	0.41
1:A:777:LEU:O	1:A:778:ARG:C	2.63	0.41
1:A:786:LEU:O	1:A:789:HIS:N	2.53	0.41
1:A:1991:ASN:O	1:A:1992:ASN:O	2.38	0.41
1:A:2010:CYS:O	1:A:2012:SER:N	2.53	0.41
1:B:883:ASP:HA	1:B:886:ARG:CB	2.50	0.41
1:B:1193:SER:O	1:B:1194:VAL:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1872:ALA:C	1:B:1874:VAL:N	2.79	0.41
1:A:522:LEU:O	1:A:523:LEU:C	2.64	0.41
1:A:762:ASP:O	1:A:763:LEU:C	2.63	0.41
1:A:838:GLU:O	1:A:839:PHE:C	2.64	0.41
1:A:972:LEU:C	1:A:974:ILE:H	2.29	0.41
1:A:1190:GLU:O	1:A:1193:SER:CB	2.69	0.41
1:A:1855:PHE:O	1:A:1857:LYS:N	2.54	0.41
1:A:1884:LYS:C	1:A:1886:LYS:N	2.79	0.41
1:A:2047:CYS:CB	1:A:2050:ASN:CB	2.99	0.41
1:B:52:LYS:C	1:B:54:ARG:N	2.78	0.41
1:B:633:TYR:O	1:B:634:LEU:C	2.63	0.41
1:B:882:SER:O	1:B:885:LEU:CB	2.68	0.41
1:B:1040:ILE:O	1:B:1041:PHE:C	2.63	0.41
1:B:1209:GLY:O	1:B:1210:ALA:C	2.64	0.41
1:B:1215:LEU:C	1:B:1219:GLN:H	2.26	0.41
1:A:660:THR:C	1:A:662:ALA:N	2.79	0.41
1:A:966:MET:C	1:A:968:MET:N	2.78	0.41
1:A:1298:CYS:O	1:A:1299:ILE:CB	2.68	0.41
1:A:1477:TYR:HA	1:A:1881:LEU:CB	2.50	0.41
1:B:18:TYR:HA	1:B:25:GLY:O	2.21	0.41
1:A:316:ALA:HA	1:A:354:SER:O	2.20	0.41
1:A:687:LEU:O	1:A:688:GLU:C	2.62	0.41
1:A:1837:THR:O	1:A:1838:ILE:C	2.62	0.41
1:B:268:GLY:C	1:B:269:ARG:O	2.64	0.41
1:B:439:GLU:O	1:B:442:ASP:CB	2.68	0.41
1:B:664:ILE:O	1:B:665:LEU:CB	2.68	0.41
1:B:1288:ASN:O	1:B:1290:ARG:N	2.53	0.41
1:B:1594:ARG:HA	1:B:1597:ARG:CB	2.50	0.41
1:B:1952:ALA:O	1:B:1953:LYS:CB	2.69	0.41
1:B:2197:ILE:HA	1:B:2212:PRO:CA	2.50	0.41
1:A:69:GLN:HA	1:A:96:ALA:HB2	2.03	0.41
1:A:398:TRP:O	1:A:399:VAL:O	2.39	0.41
1:A:704:ASN:C	1:A:706:GLU:N	2.78	0.41
1:A:743:MET:O	1:A:744:CYS:O	2.39	0.41
1:A:881:PHE:C	1:A:883:ASP:H	2.29	0.41
1:A:1001:PHE:O	1:A:1002:ASP:CB	2.67	0.41
1:A:1115:ILE:O	1:A:1116:LYS:C	2.60	0.41
1:A:1355:ILE:O	1:A:1356:GLN:CB	2.69	0.41
1:A:1477:TYR:CA	1:A:1881:LEU:CB	2.99	0.41
1:B:692:ASP:O	1:B:696:VAL:CB	2.69	0.41
1:B:776:ASP:O	1:B:778:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:LEU:C	1:B:980:PHE:N	2.76	0.41
1:B:1301:THR:O	1:B:1304:ARG:CB	2.69	0.41
1:B:1822:GLU:O	1:B:1825:LEU:CB	2.69	0.41
1:B:2052:ASN:O	1:B:2053:CYS:C	2.64	0.41
1:B:2084:VAL:O	1:B:2085:LEU:C	2.64	0.41
1:B:2147:SER:O	1:B:2151:VAL:CB	2.69	0.41
1:B:2181:GLY:O	1:B:2184:ALA:HB3	2.21	0.41
1:A:140:ALA:HB3	1:A:143:GLU:O	2.20	0.41
1:A:253:CYS:HA	1:A:262:VAL:HA	2.03	0.41
1:A:755:ILE:O	1:A:756:SER:C	2.61	0.41
1:A:773:LEU:CB	1:A:779:ALA:HB2	2.51	0.41
1:A:971:LYS:O	1:A:972:LEU:C	2.63	0.41
1:A:1812:MET:O	1:A:1814:ALA:N	2.53	0.41
1:B:105:THR:O	1:B:108:ARG:N	2.49	0.41
1:B:266:THR:HG21	1:B:1257:LYS:CB	2.51	0.41
1:B:395:THR:O	1:B:396:ASN:C	2.64	0.41
1:B:688:GLU:O	1:B:689:ALA:C	2.63	0.41
1:B:967:VAL:O	1:B:970:THR:N	2.54	0.41
1:B:974:ILE:C	1:B:976:GLU:N	2.75	0.41
1:B:989:ARG:O	1:B:990:ILE:CB	2.69	0.41
1:B:1095:GLN:O	1:B:1096:ALA:C	2.63	0.41
1:B:1975:LEU:O	1:B:1976:CYS:C	2.61	0.41
1:A:523:LEU:O	1:A:524:GLN:O	2.37	0.40
1:A:831:GLU:O	1:A:832:ARG:C	2.63	0.40
1:A:886:ARG:O	1:A:889:LYS:N	2.54	0.40
1:A:1201:GLN:O	1:A:1203:ARG:N	2.54	0.40
1:B:568:ARG:O	1:B:569:LYS:C	2.64	0.40
1:B:2157:ILE:O	1:B:2161:GLN:CB	2.68	0.40
1:A:1203:ARG:O	1:A:1207:ASN:N	2.45	0.40
1:A:1623:SER:C	1:A:1626:VAL:H	2.30	0.40
1:A:1634:LEU:CB	1:A:1646:CYS:O	2.69	0.40
1:B:1849:ASP:CB	1:B:1853:GLU:H	2.34	0.40
1:B:2071:ASN:O	1:B:2072:ASP:C	2.64	0.40
1:B:2116:ARG:O	1:B:2117:PRO:CB	2.67	0.40
1:A:896:ASP:C	1:A:898:VAL:H	2.29	0.40
1:A:1804:SER:O	1:A:1805:ASN:C	2.63	0.40
1:B:101:LYS:O	1:B:102:GLN:C	2.64	0.40
1:B:1966:GLN:HA	1:B:1969:LEU:CB	2.50	0.40
1:A:224:MET:HA	1:A:293:ARG:CB	2.52	0.40
1:A:269:ARG:CZ	2:A:3000:I3P:O52	2.68	0.40
1:A:449:ALA:O	1:A:450:SER:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:PHE:C	1:A:1003:GLU:H	2.30	0.40
1:A:1378:VAL:HA	1:A:1381:LEU:CB	2.51	0.40
1:A:1435:VAL:CB	1:A:1492:SER:CB	3.00	0.40
1:B:755:ILE:O	1:B:756:SER:C	2.65	0.40
1:B:1801:GLU:C	1:B:1802:GLY:O	2.64	0.40
1:B:1836:THR:O	1:B:1839:GLN:CB	2.69	0.40
1:B:1836:THR:CB	1:B:1984:GLN:CB	3.00	0.40
1:B:1886:LYS:O	1:B:1887:ASP:O	2.39	0.40
1:B:2069:ILE:O	1:B:2070:LEU:C	2.64	0.40
1:A:607:GLU:O	1:A:608:LYS:C	2.64	0.40
1:B:1080:LEU:O	1:B:1083:LEU:CB	2.69	0.40
1:B:1179:ILE:O	1:B:1183:LEU:CB	2.69	0.40
1:B:1235:ARG:O	1:B:1236:LEU:C	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1689/2217 (76%)	1219 (72%)	330 (20%)	140 (8%)	0	9
1	B	1688/2217 (76%)	1173 (70%)	350 (21%)	165 (10%)	0	7
All	All	3377/4434 (76%)	2392 (71%)	680 (20%)	305 (9%)	0	8

All (305) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	LEU
1	A	628	PRO
1	A	659	PRO
1	A	666	ILE
1	A	669	LYS

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Mol	Chain	Res	Type
1	A	682	THR
1	A	725	GLU
1	A	744	CYS
1	A	764	ILE
1	A	854	PHE
1	A	986	LEU
1	A	990	ILE
1	A	1119	LEU
1	A	1202	GLN
1	A	1239	GLU
1	A	1264	ASN
1	A	1288	ASN
1	A	1346	ASN
1	A	1370	PRO
1	A	1400	LEU
1	A	1418	VAL
1	A	1458	CYS
1	A	1464	THR
1	A	1637	PRO
1	A	1654	LYS
1	A	1803	ALA
1	A	1842	PHE
1	A	1859	PHE
1	A	1864	LYS
1	A	1865	VAL
1	A	1887	ASP
1	A	1993	LYS
1	A	2011	GLY
1	A	2013	THR
1	A	2046	PRO
1	A	2143	ASP
1	A	2148	PRO
1	A	2178	GLN
1	A	2190	LYS
1	A	2204	MET
1	A	2210	PRO
1	A	2215	CYS
1	B	48	ASN
1	B	591	ALA
1	B	628	PRO
1	B	659	PRO
1	B	665	LEU

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Mol	Chain	Res	Type
1	B	666	ILE
1	B	694	GLU
1	B	696	VAL
1	B	697	TRP
1	B	741	ALA
1	B	744	CYS
1	B	773	LEU
1	B	774	PRO
1	B	776	ASP
1	B	849	CYS
1	B	854	PHE
1	B	857	LYS
1	B	893	ALA
1	B	894	ILE
1	B	968	MET
1	B	982	LEU
1	B	983	ASN
1	B	990	ILE
1	B	999	ARG
1	B	1008	SER
1	B	1107	GLN
1	B	1214	VAL
1	B	1215	LEU
1	B	1220	ILE
1	B	1285	SER
1	B	1288	ASN
1	B	1300	GLU
1	B	1311	PHE
1	B	1400	LEU
1	B	1462	ASN
1	B	1463	ASN
1	B	1492	SER
1	B	1632	PRO
1	B	1637	PRO
1	B	1639	ASN
1	B	1642	ALA
1	B	1801	GLU
1	B	1850	LYS
1	B	1887	ASP
1	B	1967	PRO
1	B	1986	PHE
1	B	1987	LEU

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Mol	Chain	Res	Type
1	B	1992	ASN
1	B	2046	PRO
1	B	2075	PRO
1	B	2117	PRO
1	B	2129	MET
1	B	2194	GLN
1	B	2209	PHE
1	B	2210	PRO
1	A	225	LYS
1	A	399	VAL
1	A	412	LYS
1	A	477	LEU
1	A	550	ARG
1	A	566	ASP
1	A	578	PHE
1	A	708	ARG
1	A	726	ASP
1	A	739	LEU
1	A	858	GLU
1	A	899	HIS
1	A	983	ASN
1	A	1008	SER
1	A	1083	LEU
1	A	1208	MET
1	A	1267	ILE
1	A	1299	ILE
1	A	1347	ASP
1	A	1461	CYS
1	A	1612	ASP
1	A	1817	ASP
1	A	1820	PHE
1	A	1844	CYS
1	A	1885	LYS
1	A	1966	GLN
1	A	1984	GLN
1	A	2020	LEU
1	A	2054	ILE
1	A	2060	ASN
1	A	2104	ASP
1	A	2115	MET
1	A	2146	ALA
1	B	189	ALA

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Mol	Chain	Res	Type
1	B	236	GLY
1	B	269	ARG
1	B	552	ILE
1	B	589	VAL
1	B	612	ALA
1	B	680	VAL
1	B	681	SER
1	B	682	THR
1	B	695	GLU
1	B	703	SER
1	B	708	ARG
1	B	767	CYS
1	B	790	VAL
1	B	853	PRO
1	B	869	LEU
1	B	980	PHE
1	B	987	ASP
1	B	989	ARG
1	B	1002	ASP
1	B	1095	GLN
1	B	1116	LYS
1	B	1129	SER
1	B	1130	GLU
1	B	1239	GLU
1	B	1289	GLU
1	B	1290	ARG
1	B	1291	VAL
1	B	1388	LYS
1	B	1461	CYS
1	B	1471	ASP
1	B	1633	GLU
1	B	1817	ASP
1	B	1828	ILE
1	B	1966	GLN
1	B	2029	VAL
1	B	2178	GLN
1	B	2195	ILE
1	B	2197	ILE
1	B	2204	MET
1	A	180	ASP
1	A	521	LYS
1	A	727	ARG

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Mol	Chain	Res	Type
1	A	773	LEU
1	A	973	LYS
1	A	984	VAL
1	A	994	LEU
1	A	1028	LEU
1	A	1049	PRO
1	A	1090	ARG
1	A	1216	GLU
1	A	1349	ALA
1	A	1394	ILE
1	A	1801	GLU
1	A	1881	LEU
1	A	1992	ASN
1	A	1999	VAL
1	A	2056	THR
1	A	2062	ILE
1	A	2147	SER
1	A	2165	HIS
1	A	2189	ALA
1	A	2202	ARG
1	B	50	PRO
1	B	53	PHE
1	B	396	ASN
1	B	595	ILE
1	B	604	LYS
1	B	699	PHE
1	B	971	LYS
1	B	978	LEU
1	B	1082	LEU
1	B	1088	SER
1	B	1241	LEU
1	B	1244	PHE
1	B	1258	HIS
1	B	1405	ILE
1	B	1435	VAL
1	B	1460	ALA
1	B	1814	ALA
1	B	2012	SER
1	B	2024	ILE
1	B	2045	GLY
1	B	2060	ASN
1	B	2112	LEU

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Mol	Chain	Res	Type
1	B	2130	GLN
1	B	2146	ALA
1	B	2196	GLU
1	B	2207	ILE
1	A	606	LEU
1	A	607	GLU
1	A	685	ASN
1	A	704	ASN
1	A	719	ALA
1	A	790	VAL
1	A	1095	GLN
1	A	1630	HIS
1	A	1639	ASN
1	A	1860	TYR
1	A	1967	PRO
1	A	2150	ASN
1	B	383	PRO
1	B	640	SER
1	B	785	MET
1	B	899	HIS
1	B	993	LEU
1	B	1083	LEU
1	B	1087	PHE
1	B	1243	ASN
1	B	1268	LEU
1	B	1363	ASP
1	B	1397	ASN
1	B	1651	PHE
1	B	1953	LYS
1	B	2183	GLU
1	B	2205	GLU
1	A	383	PRO
1	A	573	TYR
1	A	661	ASN
1	A	750	LEU
1	A	763	LEU
1	A	864	PHE
1	A	871	ARG
1	A	1006	SER
1	A	1311	PHE
1	A	1414	CYS
1	A	1463	ASN

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Mol	Chain	Res	Type
1	A	1655	LEU
1	A	1662	LEU
1	A	1805	ASN
1	B	291	PRO
1	B	761	VAL
1	B	766	ARG
1	B	858	GLU
1	B	984	VAL
1	B	1247	GLY
1	B	1277	PHE
1	B	1347	ASP
1	B	1355	ILE
1	B	1356	GLN
1	B	1480	GLU
1	B	2165	HIS
1	B	2202	ARG
1	A	236	GLY
1	A	572	GLU
1	A	600	HIS
1	A	707	ILE
1	A	752	ILE
1	A	993	LEU
1	A	998	LYS
1	B	126	LEU
1	B	683	GLY
1	B	698	LEU
1	B	700	TRP
1	B	1098	LYS
1	B	1202	GLN
1	B	1286	GLU
1	B	2054	ILE
1	A	291	PRO
1	A	1109	VAL
1	A	1834	GLY
1	A	1858	VAL
1	A	1833	GLY
1	B	722	GLY
1	B	1194	VAL
1	B	2176	GLY
1	A	852	PHE
1	B	413	PRO
1	B	414	VAL

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Mol	Chain	Res	Type
1	B	627	GLU
1	B	1650	GLY
1	B	2084	VAL
1	A	645	ILE
1	A	840	VAL
1	A	2207	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	26/1980 (1%)	26 (100%)	0	100	100
1	B	26/1980 (1%)	26 (100%)	0	100	100
All	All	52/3960 (1%)	52 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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	B	3000	-	24,24,24	1.17	2 (8%)	39,39,39	1.15	4 (10%)
2	I3P	A	3000	-	24,24,24	1.15	1 (4%)	39,39,39	1.13	4 (10%)

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	B	3000	-	-	0/15/39/39	0/1/1/1
2	I3P	A	3000	-	-	0/15/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	I3P	P5-O53	-2.30	1.46	1.54
2	A	3000	I3P	P4-O42	-2.22	1.46	1.54
2	B	3000	I3P	P1-O13	-2.19	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3000	I3P	O13-P1-O12	2.52	117.24	107.80
2	A	3000	I3P	O1-P1-O11	-2.43	100.67	109.33
2	B	3000	I3P	O43-P4-O42	2.38	116.74	107.80
2	B	3000	I3P	O1-C1-C2	2.30	113.60	108.73
2	A	3000	I3P	O53-P5-O52	2.27	116.32	107.80
2	A	3000	I3P	O1-C1-C2	2.25	113.49	108.73
2	A	3000	I3P	O5-P5-O51	-2.09	101.89	109.33
2	B	3000	I3P	O53-P5-O52	2.06	115.55	107.80

There are no chirality outliers.

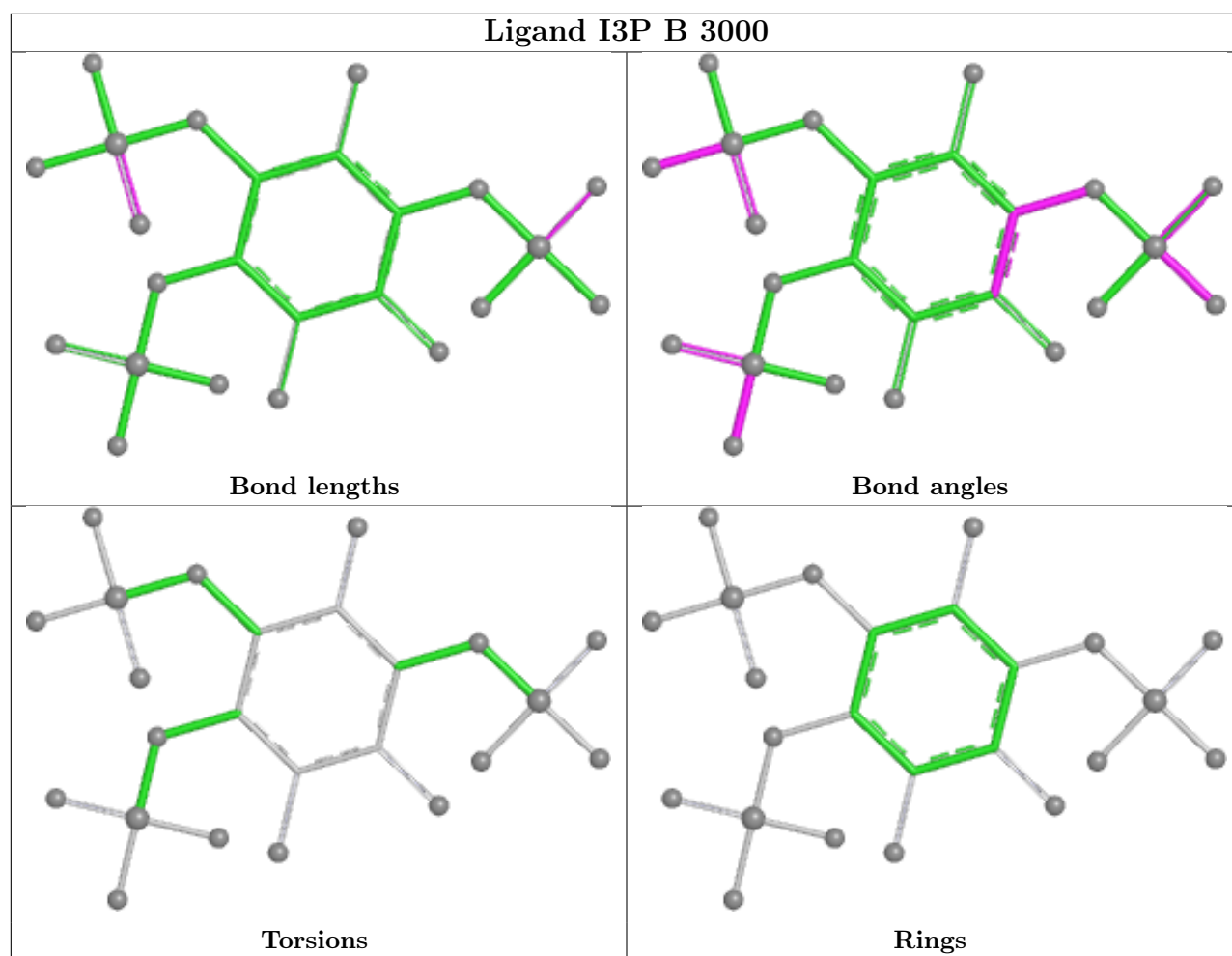
There are no torsion outliers.

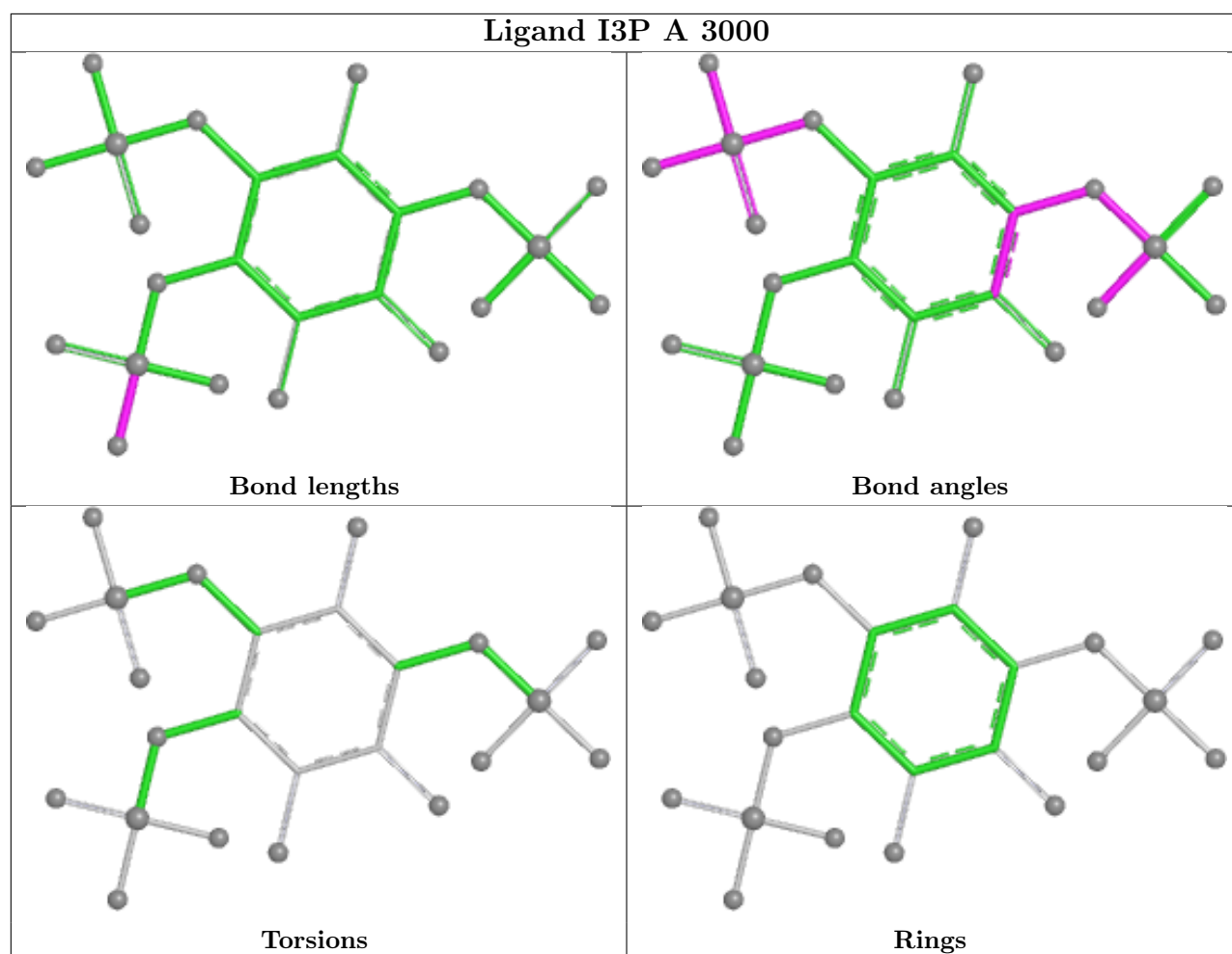
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3000	I3P	1	0
2	A	3000	I3P	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	1721/2217 (77%)	-0.40	26 (1%) 72 60	146, 167, 174, 184	0
1	B	1720/2217 (77%)	-0.38	44 (2%) 57 49	151, 166, 175, 192	0
All	All	3441/4434 (77%)	-0.39	70 (2%) 65 56	146, 166, 174, 192	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1444	ASN	6.5
1	B	1435	VAL	6.3
1	B	1443	SER	5.2
1	B	1438	LYS	5.0
1	A	548	PRO	4.8
1	B	1442	THR	4.8
1	B	1436	GLU	4.5
1	B	194	HIS	4.3
1	B	2163	ALA	4.1
1	A	147	MET	4.1
1	B	1437	MET	4.0
1	B	1439	GLU	4.0
1	B	586	GLY	3.7
1	B	1456	ASP	3.6
1	B	1370	PRO	3.5
1	B	1431	VAL	3.5
1	A	1989	CYS	3.5
1	A	136	LYS	3.2
1	B	1664	GLU	3.2
1	B	1326	CYS	3.2
1	A	35	ASP	3.1
1	B	267	THR	3.1
1	B	587	TYR	3.1
1	B	301	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	3.0
1	B	1029	ASP	3.0
1	B	168	LYS	3.0
1	A	746	ASP	2.9
1	B	2205	GLU	2.8
1	A	1096	ALA	2.8
1	A	202	ASP	2.7
1	A	283	GLU	2.6
1	A	1132	TRP	2.6
1	A	1029	ASP	2.6
1	B	1074	PRO	2.5
1	B	1113	LYS	2.5
1	B	2077	GLY	2.5
1	A	403	ASN	2.5
1	A	504	ARG	2.5
1	B	2078	LYS	2.5
1	B	2159	ALA	2.5
1	B	960	PRO	2.5
1	A	1095	GLN	2.4
1	B	1621	GLU	2.4
1	B	368	PHE	2.4
1	A	1435	VAL	2.4
1	B	167	TYR	2.4
1	A	1427	ASN	2.4
1	A	1458	CYS	2.3
1	B	462	LYS	2.3
1	B	779	ALA	2.3
1	B	1203	ARG	2.3
1	A	726	ASP	2.2
1	B	1397	ASN	2.2
1	A	1407	ARG	2.2
1	A	1889	GLU	2.2
1	B	1434	GLU	2.2
1	A	2144	GLY	2.2
1	A	1086	HIS	2.2
1	B	1815	SER	2.1
1	A	1468	LYS	2.1
1	B	83	THR	2.1
1	B	454	GLY	2.1
1	A	752	ILE	2.1
1	B	2002	THR	2.1
1	B	303	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	231	ASP	2.0
1	B	419	GLY	2.0
1	A	1488	THR	2.0
1	B	1076	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

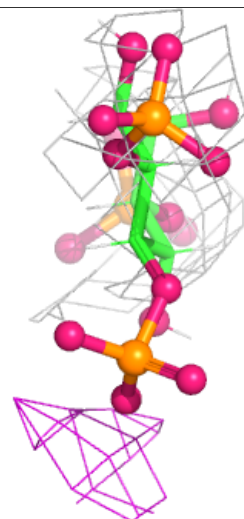
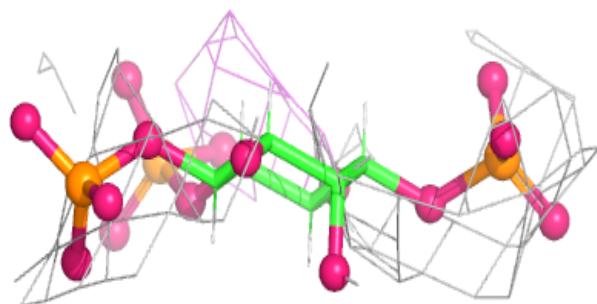
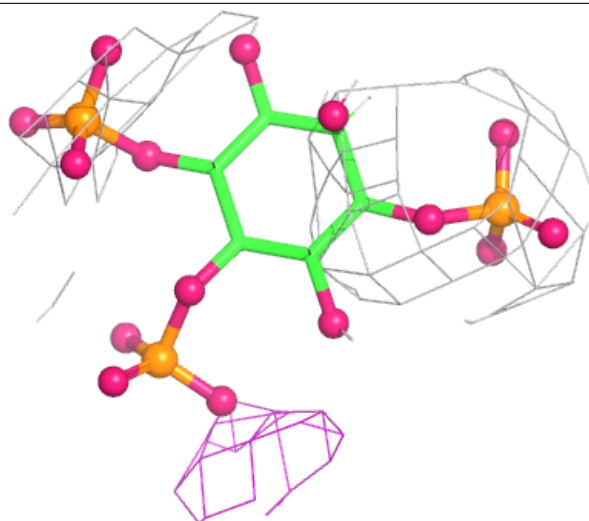
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

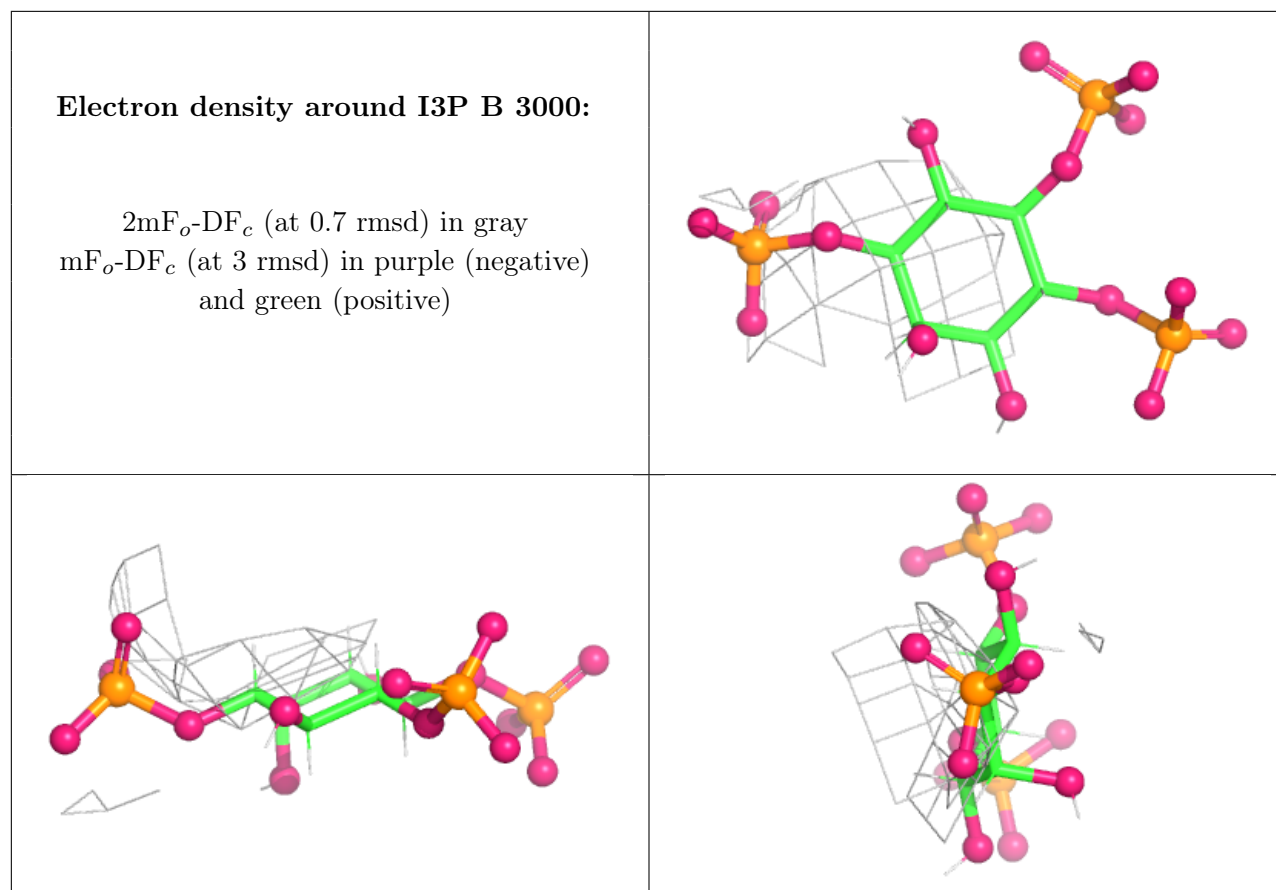
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	I3P	A	3000	24/24	0.81	0.12	169,172,172,172	0
2	I3P	B	3000	24/24	0.97	0.09	199,199,203,203	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around I3P A 3000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.