



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:05 PM UTC

PDB ID : 8WY1 / pdb_00008wy1
Title : The structure of cyclization domain in cyclic beta-1,2-glucan synthase from *Thermoanaerobacter italicus*
Authors : Tanaka, N.; Saito, R.; Kobayashi, K.; Nakai, H.; Kamo, S.; Kuramochi, K.; Taguchi, H.; Nakajima, M.; Masaike, T.
Deposited on : 2023-10-30
Resolution : 3.90 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

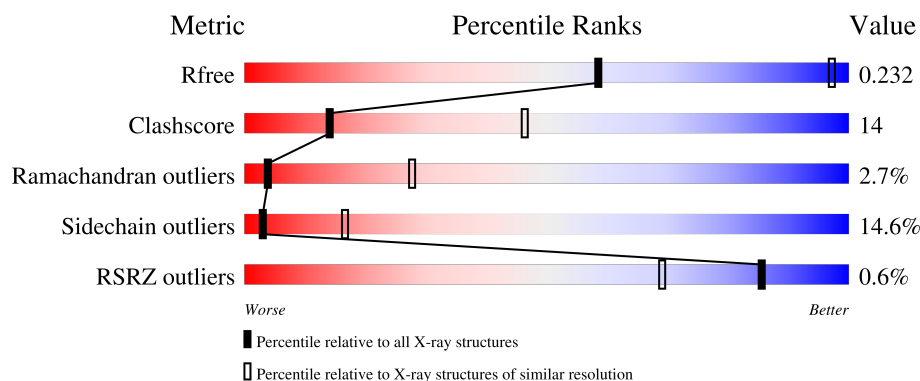
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	596	
1	B	596	
1	C	596	
1	D	596	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18842 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycosyltransferase 36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4715	3047	772	881	15			
1	B	573	Total	C	N	O	S	0	0	0
			4706	3042	771	878	15			
1	C	573	Total	C	N	O	S	0	0	0
			4706	3042	771	878	15			
1	D	574	Total	C	N	O	S	0	0	0
			4715	3047	772	881	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1004	MET	-	initiating methionine	UNP D3T4C1
A	1592	LEU	-	expression tag	UNP D3T4C1
A	1593	GLU	-	expression tag	UNP D3T4C1
A	1594	HIS	-	expression tag	UNP D3T4C1
A	1595	HIS	-	expression tag	UNP D3T4C1
A	1596	HIS	-	expression tag	UNP D3T4C1
A	1597	HIS	-	expression tag	UNP D3T4C1
A	1598	HIS	-	expression tag	UNP D3T4C1
A	1599	HIS	-	expression tag	UNP D3T4C1
B	1004	MET	-	initiating methionine	UNP D3T4C1
B	1592	LEU	-	expression tag	UNP D3T4C1
B	1593	GLU	-	expression tag	UNP D3T4C1
B	1594	HIS	-	expression tag	UNP D3T4C1
B	1595	HIS	-	expression tag	UNP D3T4C1
B	1596	HIS	-	expression tag	UNP D3T4C1
B	1597	HIS	-	expression tag	UNP D3T4C1
B	1598	HIS	-	expression tag	UNP D3T4C1
B	1599	HIS	-	expression tag	UNP D3T4C1
C	1004	MET	-	initiating methionine	UNP D3T4C1
C	1592	LEU	-	expression tag	UNP D3T4C1
C	1593	GLU	-	expression tag	UNP D3T4C1

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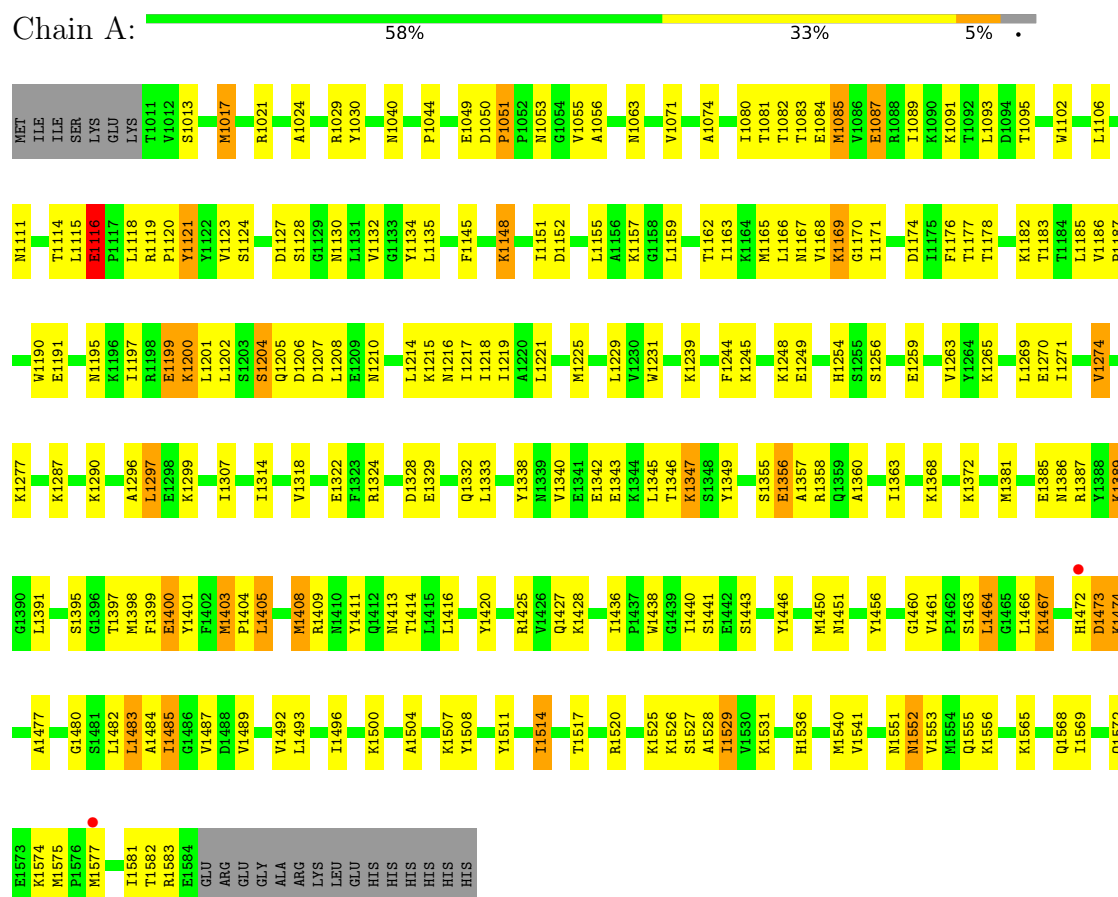
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1594	HIS	-	expression tag	UNP D3T4C1
C	1595	HIS	-	expression tag	UNP D3T4C1
C	1596	HIS	-	expression tag	UNP D3T4C1
C	1597	HIS	-	expression tag	UNP D3T4C1
C	1598	HIS	-	expression tag	UNP D3T4C1
C	1599	HIS	-	expression tag	UNP D3T4C1
D	1004	MET	-	initiating methionine	UNP D3T4C1
D	1592	LEU	-	expression tag	UNP D3T4C1
D	1593	GLU	-	expression tag	UNP D3T4C1
D	1594	HIS	-	expression tag	UNP D3T4C1
D	1595	HIS	-	expression tag	UNP D3T4C1
D	1596	HIS	-	expression tag	UNP D3T4C1
D	1597	HIS	-	expression tag	UNP D3T4C1
D	1598	HIS	-	expression tag	UNP D3T4C1
D	1599	HIS	-	expression tag	UNP D3T4C1

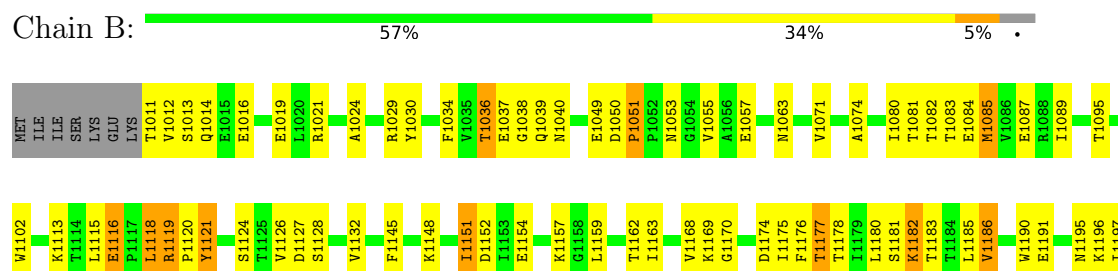
3 Residue-property plots

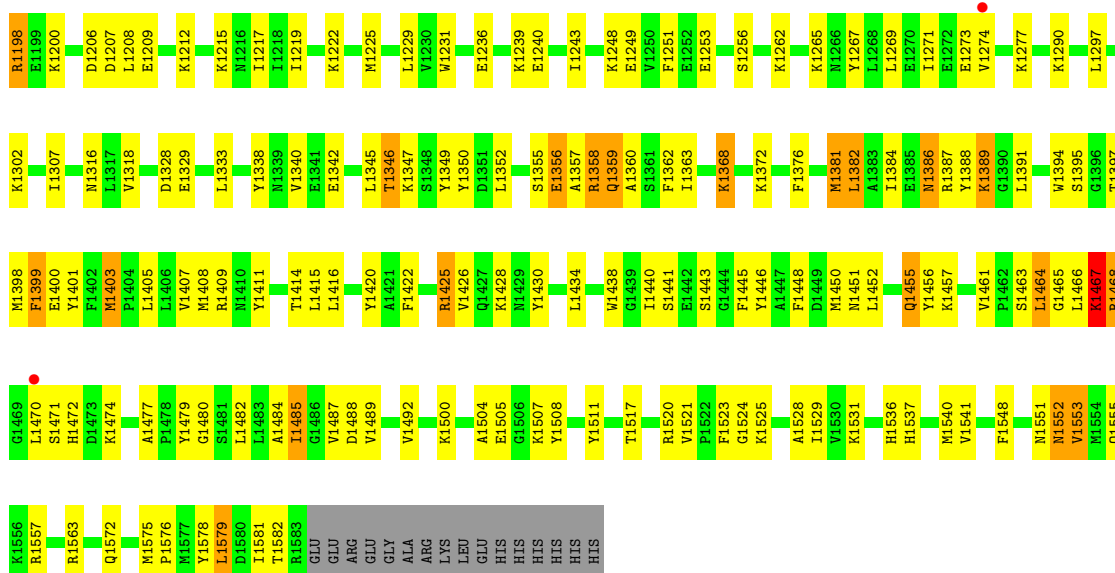
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycosyltransferase 36

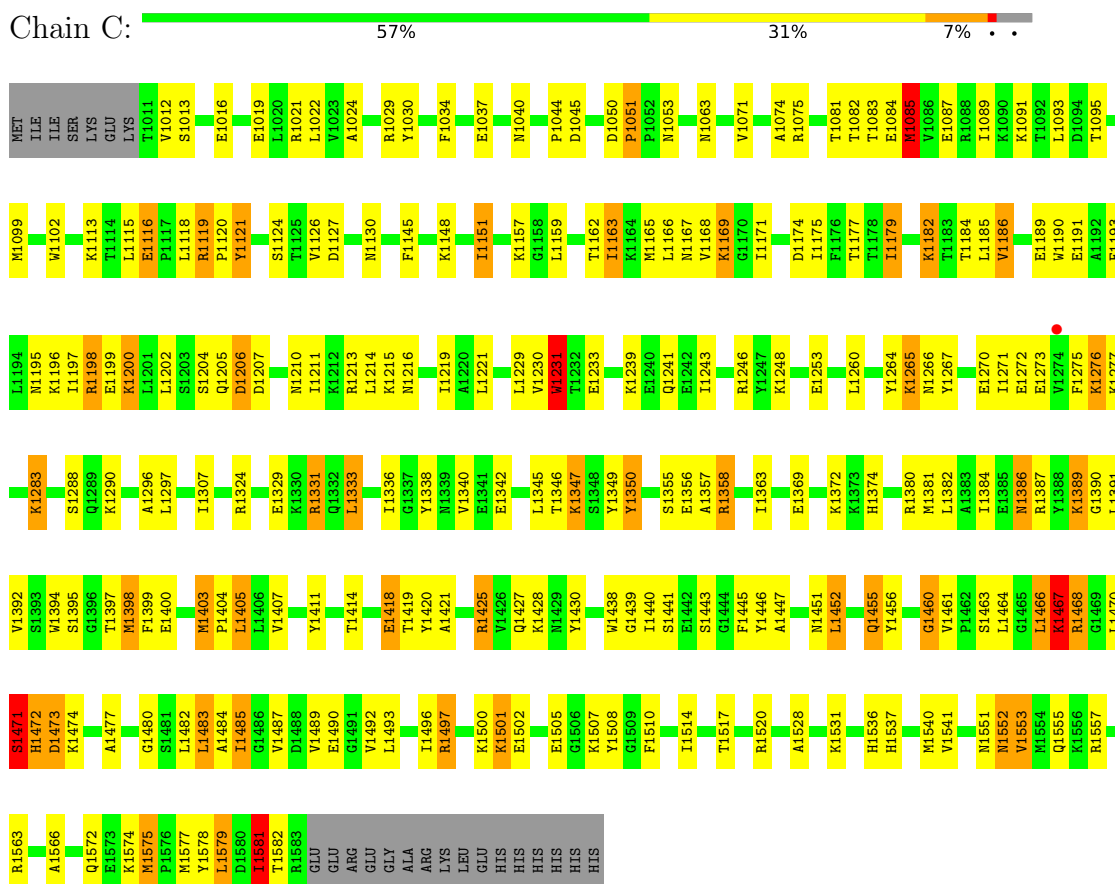


• Molecule 1: Glycosyltransferase 36





• Molecule 1: Glycosyltransferase 36



• Molecule 1: Glycosyltransferase 36



R1520	V1521	K1525	A1528	I1529	V1530	K1531	H1536	M1540	V1541	N1551	M1552	V1553	M1554	Q1555	A1556	R1557	F1558	H1559	K1565	Q1568	Q1572	M1577	Y1578	L1579	T1582	R1583	E1584	GLU	ARG	GLU	GLY	ALA	ARG	LYS	LEU	GLU	HIS	HIS	HIS	HIS											
I1436	I1440	S1441	S1442	S1443	G1444	F1445	Y1446	A1447	F1448	D1449	M1450	N1451	L1452	Q1455	Y1456	K1457	V1461	P1462	S1463	L1464	G1465	L1466	K1467	R1468	G1469	L1470	S1471	K1474	A1477	G1480	S1481	L1482	L1483	A1484	I1485	G1486	V1487	D1488	V1489	V1492	L1493	K1500	A1504	E1505	G1506	K1507	Y1508	T1517			
R1358	I1363	A1364	I1365	A1366	K1367	K1368	E1369	V1370	D1371	K1372	K1373	M1381	L1382	A1383	I1384	E1385	M1386	R1387	Y1388	K1389	G1390	L1391	W1394	S1395	M1398	F1399	M1403	P1404	L1405	L1406	V1407	M1408	R1409	Y1410	Y1411	T1414	E1418	T1419	Y1420	A1421	F1422	V1426	Q1427	K1428	N1429	Y1430	A1431	K1432	E1433	L1434	G1435
L1269	E1270	I1271	E1272	E1273	V1274	K1277	E1280	E1281	L1285	L1286	K1287	S1288	Q1289	K1290	D1291	Q1295	A1296	L1297	E1298	I1307	S1312	T1321	R1324	D1328	E1329	K1330	R1331	Q1332	L1333	Y1338	N1339	V1340	E1341	E1342	E1343	K1344	L1345	T1346	K1347	S1348	Y1349	L1352	L1353	A1354	S1355	E1356	A1357				
I1179	L1180	S1181	T1184	L1185	V1186	W1190	F1193	L1194	N1195	K1196	I1197	R1198	L1201	D1206	D1207	I1211	K1212	R1213	L1214	K1215	N1216	I1217	I1218	I1219	A1220	L1221	K1222	M1225	L1229	V1230	W1231	E1236	E1240	Q1241	E1242	I1243	F1251	H1254	E1259	K1262	V1263	Y1264	K1265	N1266	Y1267						
I1089	K1090	K1091	T1092	L1093	M1099	W1102	W1109	K1113	T1114	L1115	E1116	P1117	L1118	R1119	P1120	Y1121	S1124	T1125	V1126	D1127	S1128	Y1134	V1138	F1145	K1148	I1151	D1152	I1153	K1157	G1158	L1159	K1160	D1161	T1162	I1163	K1164	M1165	L1166	K1169	T1172	E1173	D1174	I1175	F1176	T1177	T1178					
MET	ILE	ILE	SER	LYS	LYS	T1011	V1012	S1013	Q1014	E1015	E1016	E1019	L1020	R1021	L1022	V1023	A1024	R1029	Y1030	E1037	N1040	P1044	D1045	E1049	D1050	P1051	P1052	N1053	G1054	V1055	A1056	E1057	N1063	Y1067	V1071	I1072	G1073	A1074	R1075	T1080	T1081	T1082	T1083	E1084	M1085	V1086	E1087	R1088			

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.72Å 172.72Å 395.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.60 – 3.90 89.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.60-3.90) 100.0 (89.60-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.232 0.204 , 0.232	Depositor DCC
R_{free} test set	2738 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	104.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 107.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18842	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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 ⓘ

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	0/4814	1.58	9/6485 (0.1%)
1	B	1.01	0/4805	1.61	15/6473 (0.2%)
1	C	1.02	0/4805	1.59	12/6473 (0.2%)
1	D	1.03	0/4814	1.59	7/6485 (0.1%)
All	All	1.02	0/19238	1.59	43/25916 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1280	GLU	CA-C-N	7.97	130.96	120.28
1	D	1280	GLU	C-N-CA	7.97	130.96	120.28
1	A	1152	ASP	CA-CB-CG	7.31	119.91	112.60
1	D	1050	ASP	N-CA-CB	7.11	117.14	110.39
1	B	1051	PRO	N-CA-C	-6.64	102.60	110.70
1	A	1372	LYS	CA-C-N	6.64	129.18	120.28
1	A	1372	LYS	C-N-CA	6.64	129.18	120.28
1	B	1346	THR	CA-C-N	6.52	129.85	120.79
1	B	1346	THR	C-N-CA	6.52	129.85	120.79
1	A	1051	PRO	N-CA-C	-6.50	102.77	110.70
1	C	1051	PRO	N-CA-C	-6.38	102.91	110.70
1	A	1148	LYS	CB-CA-C	6.21	116.94	109.31
1	D	1051	PRO	N-CA-C	-6.19	103.15	110.70
1	C	1231	TRP	N-CA-CB	6.18	119.20	110.12
1	C	1398	MET	CA-CB-CG	-5.92	102.25	114.10
1	C	1460	GLY	CA-C-O	-5.92	116.42	121.57
1	C	1116	GLU	CB-CA-C	5.83	116.75	108.76
1	C	1358	ARG	N-CA-C	-5.73	106.42	113.41
1	B	1372	LYS	CA-C-N	5.69	127.90	120.28
1	B	1372	LYS	C-N-CA	5.69	127.90	120.28
1	D	1116	GLU	CB-CA-C	5.68	116.55	108.76
1	B	1116	GLU	CB-CA-C	5.56	116.41	108.68
1	C	1372	LYS	CA-C-N	5.55	127.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1372	LYS	C-N-CA	5.55	127.72	120.28
1	C	1350	TYR	O-C-N	5.37	128.85	122.46
1	B	1051	PRO	CB-CA-C	5.33	117.42	110.92
1	B	1399	PHE	CA-C-O	-5.30	114.90	120.63
1	B	1219	ILE	CA-C-N	5.26	127.64	120.54
1	B	1219	ILE	C-N-CA	5.26	127.64	120.54
1	B	1356	GLU	CA-C-N	5.21	127.52	120.38
1	B	1356	GLU	C-N-CA	5.21	127.52	120.38
1	C	1051	PRO	CB-CA-C	5.19	117.25	110.92
1	A	1116	GLU	CB-CA-C	5.17	115.85	108.76
1	B	1479	TYR	CA-C-N	5.17	125.72	119.98
1	B	1479	TYR	C-N-CA	5.17	125.72	119.98
1	A	1051	PRO	CB-CA-C	5.15	117.21	110.92
1	A	1356	GLU	CA-C-N	5.15	127.17	120.28
1	A	1356	GLU	C-N-CA	5.15	127.17	120.28
1	C	1231	TRP	CB-CA-C	-5.11	102.30	110.79
1	B	1358	ARG	CB-CA-C	-5.11	102.00	110.68
1	C	1473	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	1051	PRO	CB-CA-C	5.05	117.09	110.92
1	D	1165	MET	CA-C-O	-5.03	115.54	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4715	0	4756	113	0
1	B	4706	0	4750	152	0
1	C	4706	0	4750	170	0
1	D	4715	0	4756	130	0
All	All	18842	0	19012	542	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 14.

All (542) 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:B:1036:THR:HG23	1:B:1039:GLN:HG2	1.40	1.00
1:C:1050:ASP:HB3	1:C:1051:PRO:HD3	1.51	0.93
1:B:1387:ARG:HB3	1:C:1387:ARG:HB3	1.52	0.89
1:A:1050:ASP:HB3	1:A:1051:PRO:HD3	1.59	0.83
1:B:1395:SER:OG	1:B:1400:GLU:OE2	1.99	0.78
1:B:1050:ASP:HB3	1:B:1051:PRO:HD3	1.65	0.77
1:B:1151:ILE:HD11	1:B:1225:MET:HG3	1.65	0.77
1:D:1213:ARG:HG3	1:D:1217:ILE:HD12	1.68	0.74
1:D:1050:ASP:HB3	1:D:1051:PRO:HD3	1.70	0.73
1:C:1169:LYS:HG2	1:C:1204:SER:HB2	1.69	0.72
1:B:1579:LEU:HD21	1:C:1581:ILE:HD13	1.72	0.72
1:C:1394:TRP:HD1	1:C:1467:LYS:HG2	1.55	0.72
1:B:1196:LYS:HE3	1:B:1200:LYS:HD3	1.71	0.71
1:B:1461:VAL:HB	1:B:1464:LEU:HD12	1.73	0.70
1:B:1063:ASN:OD1	1:B:1536:HIS:HB3	1.90	0.70
1:C:1051:PRO:HB3	1:C:1452:LEU:HD12	1.74	0.70
1:B:1581:ILE:HD11	1:C:1382:LEU:HG	1.72	0.70
1:B:1119:ARG:HB3	1:B:1120:PRO:HD3	1.73	0.69
1:C:1267:TYR:O	1:C:1271:ILE:HG13	1.91	0.69
1:B:1382:LEU:HG	1:C:1581:ILE:HD11	1.75	0.69
1:C:1398:MET:HE1	1:C:1438:TRP:HZ3	1.59	0.68
1:A:1461:VAL:HB	1:A:1464:LEU:HD12	1.76	0.68
1:D:1430:TYR:O	1:D:1434:LEU:HG	1.94	0.67
1:D:1461:VAL:HG13	1:D:1464:LEU:HD12	1.77	0.67
1:C:1075:ARG:HG2	1:C:1085:MET:HE2	1.76	0.66
1:D:1559:HIS:O	1:D:1565:LYS:HD3	1.95	0.66
1:A:1063:ASN:OD1	1:A:1536:HIS:HB3	1.96	0.66
1:C:1394:TRP:CD1	1:C:1467:LYS:HG2	2.31	0.66
1:C:1231:TRP:HH2	1:C:1260:LEU:HD22	1.60	0.65
1:D:1241:GLN:OE1	1:D:1286:LEU:HG	1.94	0.65
1:D:1063:ASN:OD1	1:D:1536:HIS:HB3	1.96	0.65
1:C:1470:LEU:HD13	1:D:1470:LEU:HB3	1.77	0.65
1:C:1151:ILE:HG13	1:C:1229:LEU:HD11	1.79	0.64
1:D:1500:LYS:HG2	1:D:1505:GLU:HB2	1.80	0.64
1:B:1578:TYR:HA	1:C:1382:LEU:O	1.98	0.64
1:A:1395:SER:OG	1:A:1400:GLU:OE2	2.11	0.64
1:D:1462:PRO:HG3	1:D:1470:LEU:O	1.98	0.63
1:C:1204:SER:OG	1:C:1206:ASP:OD1	2.17	0.63
1:C:1536:HIS:CD2	1:C:1537:HIS:CD2	2.87	0.63
1:C:1082:THR:HG23	1:C:1145:PHE:HB3	1.81	0.62
1:A:1472:HIS:O	1:A:1473:ASP:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1166:LEU:HD11	1:D:1213:ARG:HG2	1.82	0.62
1:C:1063:ASN:OD1	1:C:1536:HIS:HB3	1.99	0.62
1:A:1050:ASP:HB2	1:A:1531:LYS:HB2	1.82	0.62
1:D:1265:LYS:HE3	1:D:1297:LEU:HD21	1.80	0.62
1:C:1050:ASP:HB3	1:C:1051:PRO:CD	2.28	0.61
1:B:1536:HIS:CD2	1:B:1537:HIS:CD2	2.88	0.61
1:B:1394:TRP:O	1:B:1466:LEU:O	2.18	0.60
1:C:1231:TRP:CH2	1:C:1260:LEU:HD22	2.35	0.60
1:D:1050:ASP:HB2	1:D:1531:LYS:HG3	1.83	0.60
1:D:1446:TYR:CD1	1:D:1528:ALA:HB1	2.37	0.59
1:D:1216:ASN:HA	1:D:1219:ILE:HB	1.84	0.59
1:B:1576:PRO:HG2	1:C:1581:ILE:HD12	1.83	0.59
1:D:1485:ILE:HA	1:D:1492:VAL:HG21	1.85	0.59
1:D:1201:LEU:HD22	1:D:1211:ILE:HG23	1.83	0.59
1:C:1199:GLU:HA	1:C:1202:LEU:HD12	1.84	0.59
1:B:1376:PHE:HB2	1:D:1450:MET:HE3	1.85	0.59
1:C:1126:VAL:HG22	1:C:1357:ALA:HB2	1.83	0.59
1:A:1082:THR:HG23	1:A:1145:PHE:HB3	1.83	0.59
1:B:1265:LYS:HE3	1:B:1297:LEU:HD21	1.84	0.58
1:C:1446:TYR:CD1	1:C:1528:ALA:HB1	2.38	0.58
1:A:1358:ARG:NH1	1:A:1401:TYR:O	2.36	0.58
1:B:1582:THR:CG2	1:C:1380:ARG:H	2.16	0.58
1:D:1267:TYR:O	1:D:1271:ILE:HG13	2.03	0.58
1:C:1394:TRP:O	1:C:1467:LYS:HG3	2.03	0.58
1:D:1385:GLU:HB3	1:D:1422:PHE:HE1	1.68	0.58
1:A:1114:THR:OG1	1:A:1116:GLU:HB2	2.02	0.58
1:D:1082:THR:HG23	1:D:1145:PHE:HB3	1.86	0.58
1:B:1119:ARG:O	1:B:1121:TYR:N	2.36	0.58
1:C:1460:GLY:N	1:C:1468:ARG:HH21	2.02	0.58
1:B:1582:THR:HG23	1:C:1380:ARG:H	1.68	0.58
1:C:1411:TYR:HB2	1:C:1414:THR:HG21	1.86	0.57
1:C:1440:ILE:HD12	1:C:1440:ILE:H	1.69	0.57
1:A:1119:ARG:O	1:A:1121:TYR:N	2.37	0.57
1:C:1468:ARG:HD2	1:C:1471:SER:HB2	1.85	0.57
1:C:1485:ILE:HA	1:C:1492:VAL:HG21	1.85	0.57
1:D:1194:LEU:O	1:D:1198:ARG:HG2	2.04	0.57
1:B:1198:ARG:HD2	1:B:1215:LYS:HE3	1.85	0.57
1:D:1194:LEU:HD21	1:D:1221:LEU:HD13	1.86	0.57
1:A:1482:LEU:HD13	1:A:1541:VAL:HG13	1.86	0.57
1:B:1082:THR:HG23	1:B:1145:PHE:HB3	1.87	0.57
1:B:1145:PHE:HA	1:B:1148:LYS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1355:SER:O	1:B:1358:ARG:HG3	2.04	0.56
1:B:1578:TYR:CB	1:C:1381:MET:HE1	2.35	0.56
1:C:1461:VAL:HB	1:C:1464:LEU:HD12	1.87	0.56
1:C:1119:ARG:O	1:C:1121:TYR:N	2.38	0.56
1:A:1440:ILE:H	1:A:1440:ILE:HD12	1.70	0.56
1:A:1485:ILE:HA	1:A:1492:VAL:HG21	1.88	0.56
1:C:1145:PHE:HA	1:C:1148:LYS:HB2	1.88	0.56
1:A:1381:MET:O	1:A:1391:LEU:HA	2.06	0.56
1:C:1421:ALA:O	1:C:1425:ARG:HD2	2.05	0.56
1:C:1050:ASP:HB2	1:C:1531:LYS:HB2	1.88	0.56
1:A:1244:PHE:O	1:A:1248:LYS:HG3	2.06	0.55
1:D:1428:LYS:O	1:D:1432:LYS:HG3	2.05	0.55
1:A:1443:SER:HB3	1:A:1477:ALA:HB2	1.88	0.55
1:C:1130:ASN:CG	1:C:1403:MET:HE2	2.31	0.55
1:D:1353:LEU:O	1:D:1358:ARG:HD3	2.06	0.55
1:A:1151:ILE:CG1	1:A:1229:LEU:HD11	2.36	0.55
1:C:1186:VAL:HG22	1:C:1189:GLU:HG3	1.87	0.55
1:A:1187:PRO:O	1:A:1225:MET:HE1	2.07	0.55
1:A:1398:MET:HE2	1:A:1480:GLY:O	2.07	0.55
1:B:1456:TYR:O	1:B:1457:LYS:HG2	2.07	0.55
1:D:1445:PHE:CE1	1:D:1457:LYS:HG2	2.42	0.55
1:D:1387:ARG:HG2	1:D:1388:TYR:H	1.72	0.55
1:D:1448:PHE:HB3	1:D:1452:LEU:HA	1.89	0.55
1:A:1496:ILE:O	1:A:1500:LYS:HG2	2.07	0.55
1:C:1102:TRP:CZ2	1:C:1338:TYR:CD2	2.95	0.55
1:B:1124:SER:HB3	1:B:1127:ASP:HB2	1.89	0.55
1:A:1151:ILE:HG13	1:A:1229:LEU:HD11	1.87	0.54
1:B:1405:LEU:HD21	1:B:1420:TYR:CZ	2.41	0.54
1:A:1507:LYS:HD3	1:A:1508:TYR:CE2	2.43	0.54
1:C:1166:LEU:HD11	1:C:1213:ARG:HG2	1.90	0.54
1:C:1196:LYS:O	1:C:1200:LYS:HG3	2.08	0.54
1:A:1229:LEU:HD22	1:A:1231:TRP:CH2	2.42	0.54
1:A:1414:THR:HG21	1:A:1572:GLN:HA	1.89	0.54
1:B:1398:MET:HE2	1:B:1480:GLY:O	2.07	0.54
1:D:1194:LEU:HD11	1:D:1221:LEU:HB3	1.88	0.54
1:B:1267:TYR:O	1:B:1271:ILE:HG13	2.07	0.54
1:A:1416:LEU:HB3	1:A:1420:TYR:CE2	2.44	0.53
1:D:1016:GLU:O	1:D:1019:GLU:HB3	2.08	0.53
1:D:1271:ILE:HB	1:D:1290:LYS:HE3	1.89	0.53
1:C:1168:VAL:HB	1:C:1210:ASN:HD21	1.74	0.53
1:D:1124:SER:HB3	1:D:1127:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1440:ILE:HD12	1:B:1440:ILE:H	1.73	0.53
1:C:1398:MET:HE2	1:C:1480:GLY:O	2.07	0.53
1:B:1524:GLY:O	1:B:1525:LYS:HE3	2.08	0.53
1:C:1231:TRP:CZ3	1:C:1264:TYR:CE1	2.97	0.53
1:C:1382:LEU:HD22	1:C:1390:GLY:C	2.34	0.53
1:D:1075:ARG:HH21	1:D:1082:THR:HG1	1.57	0.53
1:D:1145:PHE:HA	1:D:1148:LYS:HB2	1.90	0.53
1:C:1536:HIS:HD2	1:C:1537:HIS:CD2	2.27	0.53
1:D:1440:ILE:HD12	1:D:1440:ILE:H	1.73	0.53
1:B:1466:LEU:O	1:B:1467:LYS:HB3	2.09	0.53
1:D:1254:HIS:HB3	1:D:1259:GLU:HB3	1.91	0.53
1:D:1398:MET:HE2	1:D:1480:GLY:O	2.08	0.53
1:A:1265:LYS:O	1:A:1269:LEU:HG	2.09	0.52
1:C:1496:ILE:HG23	1:C:1510:PHE:HZ	1.74	0.52
1:D:1443:SER:HB3	1:D:1477:ALA:HB2	1.90	0.52
1:B:1185:LEU:HD21	1:B:1190:TRP:CD2	2.44	0.52
1:D:1482:LEU:HD13	1:D:1541:VAL:HG13	1.90	0.52
1:B:1446:TYR:CD1	1:B:1528:ALA:HB1	2.44	0.52
1:B:1507:LYS:HD3	1:B:1508:TYR:CE2	2.45	0.52
1:C:1483:LEU:HD11	1:C:1540:MET:SD	2.50	0.52
1:B:1229:LEU:HD22	1:B:1231:TRP:CH2	2.45	0.52
1:C:1443:SER:HB3	1:C:1477:ALA:HB2	1.92	0.52
1:C:1445:PHE:CZ	1:C:1455:GLN:HB2	2.44	0.52
1:D:1489:VAL:O	1:D:1493:LEU:HG	2.09	0.52
1:A:1124:SER:HB3	1:A:1127:ASP:HB2	1.92	0.52
1:A:1489:VAL:O	1:A:1493:LEU:HG	2.09	0.52
1:B:1578:TYR:HB3	1:C:1381:MET:CE	2.40	0.52
1:A:1446:TYR:CD1	1:A:1528:ALA:HB1	2.44	0.52
1:B:1430:TYR:O	1:B:1434:LEU:HG	2.09	0.52
1:D:1483:LEU:HD11	1:D:1540:MET:SD	2.50	0.52
1:C:1507:LYS:HD3	1:C:1508:TYR:CE2	2.44	0.51
1:A:1395:SER:O	1:A:1460:GLY:HA3	2.11	0.51
1:C:1119:ARG:HB3	1:C:1120:PRO:HD3	1.92	0.51
1:D:1365:ILE:HG12	1:D:1370:VAL:HG23	1.92	0.51
1:A:1087:GLU:HG3	1:A:1091:LYS:HD2	1.91	0.51
1:B:1358:ARG:NH1	1:B:1401:TYR:O	2.44	0.51
1:C:1231:TRP:CH2	1:C:1264:TYR:HE1	2.28	0.51
1:B:1038:GLY:O	1:B:1113:LYS:HD2	2.10	0.51
1:A:1403:MET:HG3	1:A:1540:MET:CE	2.41	0.51
1:C:1016:GLU:O	1:C:1019:GLU:HB3	2.11	0.51
1:B:1384:ILE:HD11	1:C:1579:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:HIS:HB3	1:A:1259:GLU:HB3	1.93	0.51
1:D:1461:VAL:CG1	1:D:1464:LEU:HD12	2.41	0.51
1:B:1553:VAL:HG22	1:B:1557:ARG:HD2	1.92	0.50
1:C:1392:VAL:CG2	1:C:1466:LEU:HG	2.41	0.50
1:D:1414:THR:HG21	1:D:1572:GLN:HA	1.94	0.50
1:A:1270:GLU:O	1:A:1274:VAL:HG23	2.11	0.50
1:B:1578:TYR:HB3	1:C:1381:MET:HE1	1.93	0.50
1:B:1011:THR:HG22	1:B:1012:VAL:H	1.76	0.50
1:A:1050:ASP:HB2	1:A:1531:LYS:CB	2.41	0.50
1:D:1507:LYS:HD3	1:D:1508:TYR:CZ	2.46	0.50
1:A:1089:ILE:HG22	1:A:1093:LEU:HD12	1.93	0.50
1:A:1414:THR:CG2	1:A:1572:GLN:HA	2.41	0.50
1:C:1398:MET:SD	1:C:1439:GLY:HA2	2.51	0.50
1:B:1050:ASP:CB	1:B:1051:PRO:HD3	2.40	0.50
1:B:1536:HIS:HD2	1:B:1537:HIS:CD2	2.30	0.50
1:D:1446:TYR:CG	1:D:1528:ALA:HB1	2.47	0.50
1:A:1081:THR:OG1	1:A:1084:GLU:HB2	2.12	0.50
1:B:1384:ILE:HD11	1:C:1579:LEU:HD11	1.93	0.50
1:B:1415:LEU:HA	1:B:1575:MET:HG2	1.94	0.50
1:D:1231:TRP:CE3	1:D:1251:PHE:CD1	2.99	0.50
1:A:1185:LEU:HD21	1:A:1190:TRP:CD2	2.47	0.50
1:C:1163:ILE:HD11	1:C:1214:LEU:HD11	1.94	0.50
1:C:1553:VAL:HG22	1:C:1557:ARG:HD2	1.93	0.50
1:A:1191:GLU:O	1:A:1195:ASN:ND2	2.45	0.49
1:C:1231:TRP:HZ3	1:C:1264:TYR:CE1	2.30	0.49
1:A:1225:MET:HG3	1:A:1229:LEU:HD12	1.94	0.49
1:A:1347:LYS:O	1:A:1349:TYR:CE1	2.65	0.49
1:B:1102:TRP:CZ2	1:B:1338:TYR:CD2	3.00	0.49
1:B:1466:LEU:O	1:B:1467:LYS:HD2	2.12	0.49
1:C:1428:LYS:HG2	1:C:1438:TRP:CG	2.47	0.49
1:C:1443:SER:C	1:C:1456:TYR:HD1	2.21	0.49
1:C:1470:LEU:O	1:C:1472:HIS:N	2.45	0.49
1:A:1296:ALA:HA	1:A:1299:LYS:HD3	1.93	0.49
1:B:1414:THR:CG2	1:B:1572:GLN:HA	2.42	0.49
1:D:1179:ILE:HD12	1:D:1179:ILE:H	1.76	0.49
1:D:1565:LYS:HE2	1:D:1568:GLN:HE22	1.75	0.49
1:B:1050:ASP:HB3	1:B:1051:PRO:CD	2.38	0.49
1:B:1382:LEU:O	1:C:1578:TYR:HA	2.13	0.49
1:D:1265:LYS:O	1:D:1269:LEU:HG	2.13	0.49
1:B:1485:ILE:HA	1:B:1492:VAL:HG21	1.94	0.49
1:D:1403:MET:HB3	1:D:1404:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1443:SER:C	1:B:1456:TYR:HD1	2.21	0.49
1:C:1089:ILE:HG22	1:C:1093:LEU:HD12	1.93	0.49
1:C:1470:LEU:O	1:C:1471:SER:C	2.55	0.49
1:C:1482:LEU:HD13	1:C:1541:VAL:HG13	1.95	0.49
1:A:1216:ASN:HA	1:A:1219:ILE:HB	1.94	0.49
1:A:1411:TYR:HB2	1:A:1414:THR:HG21	1.95	0.49
1:B:1387:ARG:HB3	1:C:1387:ARG:HD2	1.95	0.49
1:D:1102:TRP:CZ2	1:D:1338:TYR:CD2	3.00	0.49
1:C:1468:ARG:HD2	1:C:1471:SER:CB	2.42	0.49
1:D:1120:PRO:O	1:D:1121:TYR:C	2.56	0.49
1:D:1153:ILE:HG12	1:D:1184:THR:HA	1.94	0.49
1:D:1552:ASN:O	1:D:1555:GLN:HB2	2.13	0.49
1:B:1152:ASP:OD1	1:B:1154:GLU:HB2	2.13	0.48
1:B:1191:GLU:O	1:B:1195:ASN:ND2	2.46	0.48
1:B:1036:THR:HG23	1:B:1039:GLN:CG	2.29	0.48
1:B:1036:THR:OG1	1:B:1038:GLY:N	2.44	0.48
1:B:1081:THR:OG1	1:B:1084:GLU:HB2	2.13	0.48
1:B:1388:TYR:CZ	1:B:1425:ARG:NH1	2.81	0.48
1:B:1445:PHE:HE1	1:B:1457:LYS:HG3	1.77	0.48
1:D:1553:VAL:HG22	1:D:1557:ARG:HD2	1.95	0.48
1:D:1126:VAL:HG22	1:D:1357:ALA:HB2	1.96	0.48
1:D:1385:GLU:HB3	1:D:1422:PHE:CE1	2.48	0.48
1:A:1102:TRP:CZ2	1:A:1338:TYR:CD2	3.02	0.48
1:A:1428:LYS:HG2	1:A:1438:TRP:CG	2.48	0.48
1:A:1552:ASN:O	1:A:1555:GLN:HB2	2.13	0.48
1:A:1050:ASP:HB3	1:A:1051:PRO:CD	2.36	0.48
1:B:1016:GLU:O	1:B:1019:GLU:HB3	2.12	0.48
1:C:1124:SER:HB3	1:C:1127:ASP:HB2	1.95	0.48
1:C:1169:LYS:N	1:C:1206:ASP:OD2	2.46	0.48
1:C:1185:LEU:HD21	1:C:1190:TRP:CD2	2.48	0.48
1:C:1265:LYS:HB3	1:C:1265:LYS:HE3	1.49	0.48
1:A:1095:THR:HG23	1:A:1115:LEU:HD11	1.95	0.48
1:D:1409:ARG:NH1	1:D:1411:TYR:OH	2.46	0.48
1:A:1405:LEU:HD21	1:A:1420:TYR:CZ	2.48	0.48
1:B:1414:THR:HG21	1:B:1572:GLN:HA	1.96	0.48
1:B:1470:LEU:O	1:B:1472:HIS:N	2.47	0.48
1:B:1504:ALA:HA	1:B:1529:ILE:HD13	1.96	0.48
1:B:1443:SER:HB3	1:B:1477:ALA:HB2	1.95	0.48
1:D:1267:TYR:CE2	1:D:1271:ILE:HD11	2.49	0.48
1:A:1200:LYS:HE2	1:A:1200:LYS:HB3	1.71	0.47
1:C:1169:LYS:HG2	1:C:1204:SER:CB	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1389:LYS:HB2	1:C:1575:MET:HE1	1.96	0.47
1:D:1119:ARG:O	1:D:1121:TYR:N	2.37	0.47
1:D:1347:LYS:O	1:D:1349:TYR:CE2	2.67	0.47
1:D:1517:THR:OG1	1:D:1520:ARG:NH2	2.47	0.47
1:B:1265:LYS:O	1:B:1269:LEU:HG	2.13	0.47
1:B:1428:LYS:HG2	1:B:1438:TRP:CG	2.49	0.47
1:A:1389:LYS:HG3	1:A:1575:MET:HE1	1.96	0.47
1:A:1245:LYS:HG2	1:A:1248:LYS:HE3	1.97	0.47
1:B:1236:GLU:O	1:B:1240:GLU:HG2	2.15	0.47
1:C:1191:GLU:O	1:C:1195:ASN:ND2	2.47	0.47
1:A:1443:SER:CB	1:A:1477:ALA:HB2	2.43	0.47
1:D:1394:TRP:CD1	1:D:1467:LYS:HD3	2.49	0.47
1:A:1443:SER:C	1:A:1456:TYR:HD1	2.23	0.47
1:A:1507:LYS:HD3	1:A:1508:TYR:CZ	2.49	0.47
1:A:1517:THR:OG1	1:A:1520:ARG:NH2	2.48	0.47
1:A:1119:ARG:HB3	1:A:1120:PRO:HD3	1.95	0.47
1:B:1362:PHE:CG	1:B:1408:MET:HE1	2.50	0.47
1:C:1179:ILE:HA	1:C:1182:LYS:NZ	2.30	0.47
1:D:1225:MET:HG3	1:D:1229:LEU:HD12	1.97	0.47
1:A:1355:SER:O	1:A:1357:ALA:N	2.48	0.47
1:B:1426:VAL:HG11	1:B:1463:SER:HB2	1.96	0.47
1:C:1382:LEU:HD23	1:C:1382:LEU:HA	1.74	0.47
1:D:1521:VAL:HG11	1:D:1525:LYS:O	2.13	0.47
1:C:1275:PHE:CZ	1:C:1283:LYS:HE3	2.50	0.47
1:C:1414:THR:HG21	1:C:1572:GLN:HA	1.96	0.47
1:D:1072:ILE:HD11	1:D:1138:VAL:HG13	1.96	0.47
1:A:1413:ASN:HB2	1:A:1574:LYS:HE2	1.96	0.46
1:B:1212:LYS:HE2	1:B:1212:LYS:HA	1.96	0.46
1:B:1482:LEU:HD13	1:B:1541:VAL:HG13	1.97	0.46
1:C:1552:ASN:O	1:C:1555:GLN:HB2	2.15	0.46
1:A:1197:ILE:CG2	1:A:1218:ILE:HD11	2.46	0.46
1:C:1382:LEU:CD2	1:C:1390:GLY:C	2.89	0.46
1:D:1169:LYS:HG3	1:D:1206:ASP:HB2	1.97	0.46
1:D:1445:PHE:CZ	1:D:1455:GLN:HB2	2.50	0.46
1:B:1517:THR:OG1	1:B:1520:ARG:NH2	2.48	0.46
1:C:1347:LYS:O	1:C:1349:TYR:CE2	2.68	0.46
1:A:1201:LEU:HB3	1:A:1215:LYS:HE3	1.96	0.46
1:B:1355:SER:C	1:B:1357:ALA:N	2.74	0.46
1:D:1236:GLU:O	1:D:1240:GLU:HG2	2.16	0.46
1:D:1381:MET:O	1:D:1391:LEU:HA	2.15	0.46
1:D:1411:TYR:HB2	1:D:1414:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1472:HIS:O	1:A:1474:LYS:N	2.49	0.46
1:B:1398:MET:HE3	1:B:1398:MET:HB3	1.87	0.46
1:C:1331:ARG:HB3	1:C:1333:LEU:HB2	1.98	0.46
1:C:1395:SER:OG	1:C:1400:GLU:OE1	2.29	0.46
1:C:1445:PHE:CE1	1:C:1455:GLN:HB2	2.51	0.46
1:C:1471:SER:O	1:C:1472:HIS:HB3	2.15	0.46
1:D:1263:VAL:CG1	1:D:1263:VAL:O	2.64	0.46
1:A:1358:ARG:HH12	1:A:1420:TYR:HE1	1.61	0.46
1:B:1040:ASN:HB2	1:B:1115:LEU:HD21	1.98	0.46
1:B:1231:TRP:CE2	1:B:1251:PHE:HB3	2.50	0.46
1:B:1456:TYR:C	1:B:1457:LYS:HG2	2.40	0.46
1:C:1324:ARG:HG3	1:C:1369:GLU:OE2	2.16	0.46
1:C:1517:THR:OG1	1:C:1520:ARG:NH2	2.48	0.46
1:D:1169:LYS:CG	1:D:1206:ASP:HB2	2.46	0.46
1:B:1422:PHE:O	1:B:1425:ARG:HG2	2.15	0.46
1:C:1087:GLU:HG3	1:C:1091:LYS:HD2	1.97	0.46
1:D:1263:VAL:O	1:D:1263:VAL:HG12	2.15	0.46
1:C:1095:THR:HG23	1:C:1115:LEU:HD11	1.98	0.46
1:C:1266:ASN:O	1:C:1270:GLU:HB3	2.16	0.46
1:C:1418:GLU:CD	1:C:1575:MET:HE2	2.41	0.46
1:C:1500:LYS:NZ	1:C:1505:GLU:OE2	2.48	0.46
1:D:1264:TYR:O	1:D:1297:LEU:HD22	2.15	0.46
1:C:1501:LYS:HG3	1:C:1502:GLU:N	2.31	0.46
1:B:1185:LEU:HD21	1:B:1190:TRP:CE3	2.51	0.45
1:C:1489:VAL:O	1:C:1493:LEU:HG	2.17	0.45
1:D:1029:ARG:O	1:D:1030:TYR:C	2.59	0.45
1:D:1229:LEU:HD22	1:D:1231:TRP:CH2	2.50	0.45
1:D:1559:HIS:O	1:D:1565:LYS:CD	2.62	0.45
1:A:1171:ILE:HG21	1:A:1214:LEU:CD2	2.46	0.45
1:B:1231:TRP:CD1	1:B:1231:TRP:C	2.93	0.45
1:C:1081:THR:OG1	1:C:1084:GLU:HB2	2.15	0.45
1:C:1418:GLU:OE1	1:C:1575:MET:HE2	2.15	0.45
1:B:1381:MET:HE1	1:C:1578:TYR:CB	2.46	0.45
1:B:1521:VAL:HG11	1:B:1525:LYS:O	2.17	0.45
1:A:1428:LYS:HG2	1:A:1438:TRP:CD1	2.51	0.45
1:A:1504:ALA:HA	1:A:1529:ILE:HD13	1.97	0.45
1:C:1336:ILE:HA	1:C:1350:TYR:CE2	2.51	0.45
1:A:1552:ASN:O	1:A:1556:LYS:HG3	2.17	0.45
1:B:1029:ARG:O	1:B:1030:TYR:C	2.60	0.45
1:A:1029:ARG:O	1:A:1030:TYR:C	2.59	0.45
1:C:1271:ILE:O	1:C:1275:PHE:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1185:LEU:HD21	1:D:1190:TRP:CD2	2.51	0.45
1:A:1504:ALA:HB2	1:A:1514:ILE:HD11	1.99	0.45
1:B:1071:VAL:O	1:B:1074:ALA:HB3	2.17	0.45
1:B:1355:SER:O	1:B:1357:ALA:N	2.49	0.45
1:B:1368:LYS:HE3	1:B:1563:ARG:HG2	1.99	0.45
1:C:1428:LYS:HG2	1:C:1438:TRP:CD1	2.52	0.45
1:C:1447:ALA:O	1:C:1455:GLN:HG2	2.17	0.45
1:D:1087:GLU:HG2	1:D:1091:LYS:HD2	1.97	0.45
1:C:1243:ILE:HD11	1:C:1270:GLU:HG2	1.97	0.45
1:D:1193:PHE:O	1:D:1197:ILE:HG12	2.17	0.45
1:B:1120:PRO:O	1:B:1121:TYR:C	2.60	0.45
1:B:1428:LYS:HG2	1:B:1438:TRP:CD1	2.52	0.45
1:B:1463:SER:C	1:B:1465:GLY:H	2.25	0.45
1:B:1581:ILE:CD1	1:C:1382:LEU:HG	2.42	0.45
1:C:1386:ASN:HB2	1:C:1387:ARG:H	1.68	0.44
1:D:1081:THR:OG1	1:D:1084:GLU:HB2	2.16	0.44
1:B:1080:ILE:HD12	1:B:1085:MET:HA	1.99	0.44
1:B:1195:ASN:OD1	1:B:1222:LYS:NZ	2.29	0.44
1:C:1355:SER:C	1:C:1357:ALA:N	2.75	0.44
1:D:1430:TYR:CD2	1:D:1461:VAL:HB	2.52	0.44
1:B:1448:PHE:HB3	1:B:1452:LEU:HA	1.99	0.44
1:C:1216:ASN:HA	1:C:1219:ILE:HD12	1.99	0.44
1:C:1443:SER:CB	1:C:1477:ALA:HB2	2.46	0.44
1:C:1563:ARG:O	1:C:1566:ALA:HB3	2.17	0.44
1:D:1071:VAL:O	1:D:1074:ALA:HB3	2.18	0.44
1:D:1166:LEU:HD11	1:D:1213:ARG:HD3	2.00	0.44
1:B:1095:THR:HG23	1:B:1115:LEU:HD11	2.00	0.44
1:B:1119:ARG:HD2	1:B:1119:ARG:HA	1.86	0.44
1:B:1407:VAL:O	1:B:1555:GLN:HA	2.17	0.44
1:D:1114:THR:OG1	1:D:1116:GLU:HB2	2.17	0.44
1:A:1053:ASN:ND2	1:A:1451:ASN:O	2.51	0.44
1:A:1145:PHE:HA	1:A:1148:LYS:HB2	1.99	0.44
1:A:1355:SER:C	1:A:1357:ALA:N	2.75	0.44
1:B:1355:SER:HA	1:B:1400:GLU:HG2	1.99	0.44
1:A:1398:MET:HE3	1:A:1398:MET:HB3	1.81	0.44
1:B:1381:MET:HE3	1:B:1381:MET:HB3	1.69	0.44
1:D:1583:ARG:O	1:D:1584:GLU:C	2.61	0.44
1:A:1111:ASN:N	1:A:1118:LEU:HD21	2.33	0.44
1:A:1159:LEU:O	1:A:1162:THR:HB	2.18	0.44
1:A:1358:ARG:NE	1:A:1404:PRO:HG2	2.33	0.44
1:B:1381:MET:CE	1:C:1578:TYR:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1445:PHE:CE1	1:B:1457:LYS:HG3	2.53	0.44
1:C:1405:LEU:HD21	1:C:1420:TYR:CZ	2.53	0.44
1:D:1053:ASN:ND2	1:D:1451:ASN:O	2.48	0.44
1:D:1355:SER:C	1:D:1357:ALA:N	2.76	0.44
1:A:1408:MET:HE3	1:A:1408:MET:HB3	1.76	0.44
1:B:1126:VAL:HG23	1:B:1350:TYR:CE2	2.53	0.44
1:B:1411:TYR:HB2	1:B:1414:THR:HG21	2.00	0.44
1:D:1331:ARG:HB3	1:D:1333:LEU:HB2	2.00	0.44
1:B:1328:ASP:O	1:B:1329:GLU:C	2.61	0.43
1:B:1381:MET:O	1:B:1391:LEU:HA	2.18	0.43
1:C:1029:ARG:O	1:C:1030:TYR:C	2.59	0.43
1:D:1040:ASN:HB2	1:D:1115:LEU:HD21	2.00	0.43
1:B:1552:ASN:O	1:B:1555:GLN:HB2	2.16	0.43
1:C:1050:ASP:HB2	1:C:1531:LYS:CB	2.47	0.43
1:C:1381:MET:O	1:C:1391:LEU:HA	2.18	0.43
1:D:1408:MET:HB3	1:D:1408:MET:HE3	1.79	0.43
1:A:1287:LYS:HD2	1:A:1287:LYS:HA	1.85	0.43
1:B:1051:PRO:HG2	1:B:1448:PHE:HE2	1.82	0.43
1:B:1536:HIS:O	1:B:1540:MET:HG3	2.18	0.43
1:C:1030:TYR:O	1:C:1034:PHE:HD2	2.01	0.43
1:C:1190:TRP:HZ2	1:C:1221:LEU:HD22	1.82	0.43
1:D:1050:ASP:HB3	1:D:1051:PRO:CD	2.45	0.43
1:D:1109:TRP:HB3	1:D:1118:LEU:HG	2.00	0.43
1:A:1021:ARG:O	1:A:1024:ALA:HB3	2.19	0.43
1:A:1044:PRO:HB2	1:A:1056:ALA:O	2.18	0.43
1:A:1169:LYS:N	1:A:1206:ASP:OD2	2.52	0.43
1:A:1265:LYS:HG3	1:A:1297:LEU:HD21	1.99	0.43
1:B:1159:LEU:O	1:B:1162:THR:HB	2.19	0.43
1:B:1581:ILE:HD11	1:C:1382:LEU:CG	2.44	0.43
1:C:1071:VAL:O	1:C:1074:ALA:HB3	2.17	0.43
1:C:1243:ILE:HA	1:C:1246:ARG:CZ	2.48	0.43
1:C:1536:HIS:CD2	1:C:1537:HIS:N	2.85	0.43
1:A:1080:ILE:HD12	1:A:1085:MET:HA	2.01	0.43
1:A:1322:GLU:HG2	1:A:1324:ARG:HH21	1.83	0.43
1:C:1185:LEU:HD21	1:C:1190:TRP:CE3	2.53	0.43
1:D:1153:ILE:CG1	1:D:1184:THR:HA	2.49	0.43
1:D:1443:SER:CB	1:D:1477:ALA:HB2	2.48	0.43
1:A:1132:VAL:HG13	1:A:1318:VAL:HG13	2.01	0.43
1:D:1394:TRP:NE1	1:D:1467:LYS:HD3	2.34	0.43
1:D:1409:ARG:HG3	1:D:1559:HIS:CE1	2.53	0.43
1:C:1358:ARG:CZ	1:C:1404:PRO:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1414:THR:CG2	1:C:1572:GLN:HA	2.49	0.43
1:D:1179:ILE:HG23	1:D:1185:LEU:HD13	2.01	0.43
1:D:1185:LEU:HD21	1:D:1190:TRP:CE3	2.54	0.43
1:A:1484:ALA:O	1:A:1485:ILE:C	2.62	0.43
1:B:1381:MET:HE1	1:C:1578:TYR:HB3	2.01	0.43
1:B:1536:HIS:CD2	1:B:1537:HIS:N	2.87	0.43
1:C:1050:ASP:HB2	1:C:1531:LYS:HG3	2.01	0.43
1:D:1190:TRP:HZ2	1:D:1221:LEU:HD22	1.84	0.43
1:D:1287:LYS:O	1:D:1291:ASP:OD1	2.37	0.43
1:D:1398:MET:HE3	1:D:1398:MET:HB3	1.80	0.43
1:A:1231:TRP:CD1	1:A:1231:TRP:C	2.97	0.42
1:B:1445:PHE:CZ	1:B:1455:GLN:HB3	2.54	0.42
1:D:1241:GLN:HG3	1:D:1289:GLN:HE22	1.84	0.42
1:A:1029:ARG:HD2	1:A:1165:MET:SD	2.59	0.42
1:A:1245:LYS:HA	1:A:1248:LYS:HD2	2.00	0.42
1:B:1397:THR:HB	1:B:1441:SER:OG	2.18	0.42
1:C:1264:TYR:HE2	1:C:1296:ALA:HB3	1.84	0.42
1:D:1021:ARG:O	1:D:1024:ALA:HB3	2.19	0.42
1:B:1208:LEU:O	1:B:1212:LYS:HG2	2.20	0.42
1:B:1403:MET:SD	1:B:1540:MET:CE	3.07	0.42
1:B:1443:SER:CB	1:B:1477:ALA:HB2	2.49	0.42
1:B:1500:LYS:NZ	1:B:1505:GLU:OE2	2.47	0.42
1:C:1175:ILE:HG22	1:C:1193:PHE:CE1	2.55	0.42
1:D:1044:PRO:O	1:D:1045:ASP:C	2.62	0.42
1:A:1155:LEU:HD22	1:A:1221:LEU:HD21	2.02	0.42
1:B:1151:ILE:HG13	1:B:1229:LEU:HD11	2.00	0.42
1:C:1053:ASN:ND2	1:C:1451:ASN:O	2.52	0.42
1:C:1333:LEU:HD23	1:C:1374:HIS:HE1	1.85	0.42
1:D:1067:TYR:OH	1:D:1088:ARG:HB3	2.20	0.42
1:D:1134:TYR:OH	1:D:1403:MET:HE2	2.20	0.42
1:D:1243:ILE:HD11	1:D:1270:GLU:C	2.45	0.42
1:A:1403:MET:HE2	1:A:1540:MET:HE1	2.00	0.42
1:C:1198:ARG:O	1:C:1202:LEU:HG	2.20	0.42
1:C:1398:MET:HE1	1:C:1438:TRP:CZ3	2.46	0.42
1:C:1497:ARG:H	1:C:1497:ARG:HG2	1.56	0.42
1:A:1040:ASN:HB2	1:A:1115:LEU:HD21	2.02	0.42
1:A:1166:LEU:O	1:A:1210:ASN:ND2	2.53	0.42
1:A:1413:ASN:CB	1:A:1574:LYS:HE2	2.50	0.42
1:B:1362:PHE:CD2	1:B:1408:MET:HE1	2.55	0.42
1:D:1291:ASP:O	1:D:1295:GLN:OE1	2.37	0.42
1:A:1085:MET:HE2	1:A:1085:MET:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1347:LYS:O	1:B:1349:TYR:CE1	2.72	0.42
1:C:1021:ARG:O	1:C:1024:ALA:HB3	2.19	0.42
1:C:1271:ILE:HB	1:C:1290:LYS:HE2	2.02	0.42
1:D:1222:LYS:HE3	1:D:1225:MET:HE1	2.02	0.42
1:B:1053:ASN:ND2	1:B:1451:ASN:O	2.52	0.42
1:B:1484:ALA:O	1:B:1485:ILE:C	2.63	0.42
1:C:1345:LEU:HD23	1:C:1345:LEU:HA	1.85	0.42
1:C:1389:LYS:HD2	1:C:1575:MET:CE	2.49	0.42
1:C:1398:MET:HG3	1:C:1427:GLN:NE2	2.35	0.42
1:D:1215:LYS:O	1:D:1219:ILE:N	2.50	0.42
1:B:1345:LEU:HD23	1:B:1345:LEU:HA	1.85	0.42
1:C:1119:ARG:HA	1:C:1119:ARG:HD2	1.88	0.42
1:C:1229:LEU:HD22	1:C:1231:TRP:CZ2	2.54	0.42
1:D:1504:ALA:HA	1:D:1529:ILE:HD13	2.01	0.42
1:A:1511:TYR:CD1	1:A:1531:LYS:HA	2.55	0.41
1:B:1389:LYS:HG3	1:B:1575:MET:CE	2.49	0.41
1:C:1179:ILE:H	1:C:1179:ILE:HD12	1.85	0.41
1:C:1407:VAL:O	1:C:1555:GLN:HA	2.20	0.41
1:C:1430:TYR:CG	1:C:1461:VAL:HG13	2.55	0.41
1:D:1385:GLU:O	1:D:1386:ASN:C	2.63	0.41
1:A:1483:LEU:HD11	1:A:1540:MET:SD	2.60	0.41
1:B:1012:VAL:HG13	1:B:1016:GLU:HB2	2.01	0.41
1:C:1271:ILE:CG2	1:C:1290:LYS:HE3	2.50	0.41
1:A:1197:ILE:HG22	1:A:1218:ILE:CD1	2.50	0.41
1:D:1383:ALA:O	1:D:1389:LYS:HA	2.20	0.41
1:D:1405:LEU:HD21	1:D:1420:TYR:CZ	2.55	0.41
1:D:1089:ILE:HG22	1:D:1093:LEU:HD12	2.02	0.41
1:D:1159:LEU:O	1:D:1162:THR:HB	2.20	0.41
1:D:1193:PHE:O	1:D:1196:LYS:HB3	2.21	0.41
1:B:1359:GLN:O	1:B:1363:ILE:HD12	2.21	0.41
1:C:1231:TRP:HH2	1:C:1264:TYR:HE1	1.69	0.41
1:C:1355:SER:C	1:C:1357:ALA:H	2.28	0.41
1:A:1071:VAL:O	1:A:1074:ALA:HB3	2.19	0.41
1:B:1050:ASP:HB2	1:B:1531:LYS:HG3	2.02	0.41
1:B:1425:ARG:HG2	1:B:1425:ARG:H	1.76	0.41
1:C:1264:TYR:HB3	1:C:1297:LEU:HD22	2.03	0.41
1:D:1080:ILE:HD12	1:D:1085:MET:HA	2.03	0.41
1:B:1273:GLU:OE1	1:B:1273:GLU:HA	2.20	0.41
1:B:1511:TYR:CD1	1:B:1531:LYS:HA	2.55	0.41
1:C:1395:SER:HB2	1:C:1468:ARG:HH22	1.86	0.41
1:D:1407:VAL:O	1:D:1555:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1190:TRP:HZ2	1:A:1221:LEU:HD22	1.86	0.41
1:B:1132:VAL:HG13	1:B:1318:VAL:HG13	2.01	0.41
1:B:1182:LYS:HE2	1:B:1186:VAL:HG13	2.02	0.41
1:B:1428:LYS:NZ	1:B:1488:ASP:OD2	2.43	0.41
1:C:1082:THR:CG2	1:C:1145:PHE:HB3	2.49	0.41
1:A:1357:ALA:O	1:A:1360:ALA:HB3	2.21	0.41
1:B:1030:TYR:O	1:B:1034:PHE:HD2	2.04	0.41
1:B:1118:LEU:HA	1:B:1118:LEU:HD22	1.89	0.41
1:B:1357:ALA:O	1:B:1360:ALA:HB3	2.21	0.41
1:B:1386:ASN:HB2	1:B:1387:ARG:H	1.69	0.41
1:C:1040:ASN:HB2	1:C:1115:LEU:HD21	2.02	0.41
1:C:1044:PRO:O	1:C:1045:ASP:C	2.64	0.41
1:C:1391:LEU:HB2	1:C:1419:THR:HG21	2.03	0.41
1:C:1397:THR:HB	1:C:1441:SER:OG	2.21	0.41
1:C:1484:ALA:O	1:C:1485:ILE:C	2.63	0.41
1:B:1071:VAL:HG11	1:B:1089:ILE:HG13	2.02	0.41
1:B:1446:TYR:CG	1:B:1528:ALA:HB1	2.56	0.41
1:C:1159:LEU:O	1:C:1162:THR:HB	2.21	0.41
1:D:1328:ASP:O	1:D:1329:GLU:C	2.64	0.41
1:D:1344:LYS:HB2	1:D:1344:LYS:HE2	1.81	0.41
1:A:1199:GLU:HA	1:A:1202:LEU:HD12	2.03	0.40
1:A:1355:SER:H	1:A:1358:ARG:HD3	1.86	0.40
1:B:1021:ARG:O	1:B:1024:ALA:HB3	2.21	0.40
1:B:1177:THR:O	1:B:1181:SER:OG	2.36	0.40
1:C:1120:PRO:O	1:C:1121:TYR:C	2.65	0.40
1:D:1160:LYS:HA	1:D:1176:PHE:CZ	2.56	0.40
1:D:1324:ARG:HG3	1:D:1369:GLU:OE2	2.20	0.40
1:A:1135:LEU:HB3	1:A:1314:ILE:HG23	2.02	0.40
1:B:1176:PHE:HB3	1:B:1180:LEU:HG	2.03	0.40
1:B:1384:ILE:CD1	1:C:1579:LEU:HD21	2.51	0.40
1:C:1126:VAL:HG23	1:C:1350:TYR:CE2	2.56	0.40
1:C:1193:PHE:CE2	1:C:1197:ILE:HD11	2.56	0.40
1:D:1484:ALA:O	1:D:1485:ILE:C	2.63	0.40
1:A:1120:PRO:O	1:A:1121:TYR:C	2.65	0.40
1:A:1130:ASN:HB3	1:A:1134:TYR:CE2	2.57	0.40
1:A:1169:LYS:HB3	1:A:1204:SER:HB2	2.03	0.40
1:A:1398:MET:HG2	1:A:1427:GLN:NE2	2.35	0.40
1:B:1485:ILE:HG12	1:B:1548:PHE:CD1	2.57	0.40
1:C:1273:GLU:HA	1:C:1276:LYS:HE2	2.03	0.40
1:D:1422:PHE:O	1:D:1426:VAL:HG23	2.21	0.40
1:A:1017:MET:HE3	1:A:1017:MET:HB2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1011:THR:HG22	1:B:1012:VAL:N	2.36	0.40
1:C:1029:ARG:HD2	1:C:1165:MET:SD	2.62	0.40
1:C:1392:VAL:HG21	1:C:1466:LEU:HG	2.02	0.40
1:A:1328:ASP:O	1:A:1329:GLU:C	2.64	0.40
1:A:1397:THR:HB	1:A:1441:SER:OG	2.22	0.40
1:B:1416:LEU:HB3	1:B:1420:TYR:CE2	2.55	0.40
1:C:1230:VAL:O	1:C:1233:GLU:HB2	2.20	0.40
1:D:1321:THR:O	1:D:1367:LYS:NZ	2.48	0.40
1:D:1485:ILE:HG23	1:D:1486:GLY:N	2.36	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	572/596 (96%)	478 (84%)	79 (14%)	15 (3%)	4	28
1	B	571/596 (96%)	483 (85%)	74 (13%)	14 (2%)	4	29
1	C	571/596 (96%)	468 (82%)	88 (15%)	15 (3%)	4	28
1	D	572/596 (96%)	463 (81%)	91 (16%)	18 (3%)	3	25
All	All	2286/2384 (96%)	1892 (83%)	332 (14%)	62 (3%)	4	28

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1356	GLU
1	A	1473	ASP
1	B	1356	GLU
1	B	1471	SER
1	C	1356	GLU
1	C	1582	THR

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Mol	Chain	Res	Type
1	D	1356	GLU
1	A	1167	ASN
1	A	1170	GLY
1	A	1177	THR
1	A	1551	ASN
1	B	1177	THR
1	B	1207	ASP
1	B	1551	ASN
1	B	1552	ASN
1	C	1471	SER
1	C	1551	ASN
1	C	1552	ASN
1	C	1581	ILE
1	D	1121	TYR
1	D	1177	THR
1	D	1386	ASN
1	D	1471	SER
1	D	1551	ASN
1	D	1578	TYR
1	A	1121	TYR
1	A	1552	ASN
1	B	1121	TYR
1	B	1206	ASP
1	B	1467	LYS
1	C	1121	TYR
1	C	1177	THR
1	D	1343	GLU
1	D	1468	ARG
1	D	1469	GLY
1	D	1552	ASN
1	D	1583	ARG
1	A	1178	THR
1	A	1207	ASP
1	C	1167	ASN
1	C	1207	ASP
1	C	1487	VAL
1	D	1207	ASP
1	A	1085	MET
1	A	1176	PHE
1	A	1467	LYS
1	A	1487	VAL
1	A	1527	SER

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Mol	Chain	Res	Type
1	B	1085	MET
1	B	1178	THR
1	B	1468	ARG
1	C	1179	ILE
1	C	1241	GLN
1	C	1467	LYS
1	D	1085	MET
1	D	1178	THR
1	D	1487	VAL
1	B	1487	VAL
1	C	1085	MET
1	D	1287	LYS
1	B	1170	GLY
1	D	1384	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/532 (96%)	436 (85%)	76 (15%)	3	16
1	B	511/532 (96%)	445 (87%)	66 (13%)	4	20
1	C	511/532 (96%)	436 (85%)	75 (15%)	3	16
1	D	512/532 (96%)	431 (84%)	81 (16%)	2	15
All	All	2046/2128 (96%)	1748 (85%)	298 (15%)	3	16

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	SER
1	A	1017	MET
1	A	1049	GLU
1	A	1055	VAL
1	A	1083	THR
1	A	1087	GLU
1	A	1106	LEU

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Mol	Chain	Res	Type
1	A	1116	GLU
1	A	1123	VAL
1	A	1128	SER
1	A	1157	LYS
1	A	1163	ILE
1	A	1168	VAL
1	A	1169	LYS
1	A	1174	ASP
1	A	1182	LYS
1	A	1183	THR
1	A	1186	VAL
1	A	1199	GLU
1	A	1200	LYS
1	A	1204	SER
1	A	1205	GLN
1	A	1208	LEU
1	A	1217	ILE
1	A	1239	LYS
1	A	1249	GLU
1	A	1256	SER
1	A	1263	VAL
1	A	1271	ILE
1	A	1274	VAL
1	A	1277	LYS
1	A	1290	LYS
1	A	1297	LEU
1	A	1307	ILE
1	A	1332	GLN
1	A	1333	LEU
1	A	1340	VAL
1	A	1342	GLU
1	A	1343	GLU
1	A	1345	LEU
1	A	1346	THR
1	A	1347	LYS
1	A	1363	ILE
1	A	1368	LYS
1	A	1385	GLU
1	A	1386	ASN
1	A	1387	ARG
1	A	1389	LYS
1	A	1399	PHE

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Mol	Chain	Res	Type
1	A	1400	GLU
1	A	1403	MET
1	A	1405	LEU
1	A	1408	MET
1	A	1409	ARG
1	A	1425	ARG
1	A	1436	ILE
1	A	1450	MET
1	A	1463	SER
1	A	1464	LEU
1	A	1466	LEU
1	A	1467	LYS
1	A	1474	LYS
1	A	1483	LEU
1	A	1485	ILE
1	A	1514	ILE
1	A	1525	LYS
1	A	1526	LYS
1	A	1529	ILE
1	A	1553	VAL
1	A	1565	LYS
1	A	1568	GLN
1	A	1569	ILE
1	A	1577	MET
1	A	1581	ILE
1	A	1582	THR
1	A	1583	ARG
1	B	1013	SER
1	B	1014	GLN
1	B	1036	THR
1	B	1037	GLU
1	B	1049	GLU
1	B	1055	VAL
1	B	1057	GLU
1	B	1083	THR
1	B	1087	GLU
1	B	1116	GLU
1	B	1118	LEU
1	B	1119	ARG
1	B	1128	SER
1	B	1151	ILE
1	B	1157	LYS

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Mol	Chain	Res	Type
1	B	1163	ILE
1	B	1168	VAL
1	B	1169	LYS
1	B	1174	ASP
1	B	1175	ILE
1	B	1182	LYS
1	B	1183	THR
1	B	1186	VAL
1	B	1197	ILE
1	B	1198	ARG
1	B	1209	GLU
1	B	1217	ILE
1	B	1239	LYS
1	B	1243	ILE
1	B	1248	LYS
1	B	1249	GLU
1	B	1253	GLU
1	B	1256	SER
1	B	1262	LYS
1	B	1274	VAL
1	B	1277	LYS
1	B	1290	LYS
1	B	1302	LYS
1	B	1307	ILE
1	B	1316	ASN
1	B	1333	LEU
1	B	1340	VAL
1	B	1342	GLU
1	B	1346	THR
1	B	1352	LEU
1	B	1359	GLN
1	B	1368	LYS
1	B	1381	MET
1	B	1382	LEU
1	B	1386	ASN
1	B	1389	LYS
1	B	1399	PHE
1	B	1403	MET
1	B	1409	ARG
1	B	1425	ARG
1	B	1450	MET
1	B	1455	GLN

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Mol	Chain	Res	Type
1	B	1464	LEU
1	B	1467	LYS
1	B	1468	ARG
1	B	1474	LYS
1	B	1485	ILE
1	B	1489	VAL
1	B	1523	PHE
1	B	1553	VAL
1	B	1579	LEU
1	C	1012	VAL
1	C	1013	SER
1	C	1022	LEU
1	C	1037	GLU
1	C	1083	THR
1	C	1085	MET
1	C	1099	MET
1	C	1113	LYS
1	C	1116	GLU
1	C	1118	LEU
1	C	1119	ARG
1	C	1151	ILE
1	C	1157	LYS
1	C	1163	ILE
1	C	1169	LYS
1	C	1171	ILE
1	C	1174	ASP
1	C	1182	LYS
1	C	1184	THR
1	C	1186	VAL
1	C	1198	ARG
1	C	1200	LYS
1	C	1205	GLN
1	C	1206	ASP
1	C	1211	ILE
1	C	1215	LYS
1	C	1231	TRP
1	C	1239	LYS
1	C	1248	LYS
1	C	1253	GLU
1	C	1265	LYS
1	C	1272	GLU
1	C	1276	LYS

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Mol	Chain	Res	Type
1	C	1277	LYS
1	C	1283	LYS
1	C	1288	SER
1	C	1307	ILE
1	C	1329	GLU
1	C	1331	ARG
1	C	1333	LEU
1	C	1340	VAL
1	C	1342	GLU
1	C	1346	THR
1	C	1347	LYS
1	C	1363	ILE
1	C	1384	ILE
1	C	1386	ASN
1	C	1389	LYS
1	C	1399	PHE
1	C	1403	MET
1	C	1405	LEU
1	C	1418	GLU
1	C	1425	ARG
1	C	1452	LEU
1	C	1455	GLN
1	C	1463	SER
1	C	1466	LEU
1	C	1467	LYS
1	C	1468	ARG
1	C	1471	SER
1	C	1472	HIS
1	C	1473	ASP
1	C	1474	LYS
1	C	1483	LEU
1	C	1485	ILE
1	C	1490	GLU
1	C	1497	ARG
1	C	1501	LYS
1	C	1514	ILE
1	C	1553	VAL
1	C	1574	LYS
1	C	1575	MET
1	C	1577	MET
1	C	1579	LEU
1	C	1581	ILE

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Mol	Chain	Res	Type
1	D	1013	SER
1	D	1015	GLU
1	D	1020	LEU
1	D	1022	LEU
1	D	1037	GLU
1	D	1049	GLU
1	D	1055	VAL
1	D	1057	GLU
1	D	1083	THR
1	D	1099	MET
1	D	1113	LYS
1	D	1116	GLU
1	D	1118	LEU
1	D	1119	ARG
1	D	1128	SER
1	D	1151	ILE
1	D	1157	LYS
1	D	1163	ILE
1	D	1169	LYS
1	D	1172	THR
1	D	1174	ASP
1	D	1175	ILE
1	D	1181	SER
1	D	1186	VAL
1	D	1206	ASP
1	D	1212	LYS
1	D	1213	ARG
1	D	1219	ILE
1	D	1236	GLU
1	D	1262	LYS
1	D	1265	LYS
1	D	1272	GLU
1	D	1277	LYS
1	D	1281	GLU
1	D	1285	LEU
1	D	1287	LYS
1	D	1291	ASP
1	D	1298	GLU
1	D	1307	ILE
1	D	1312	SER
1	D	1331	ARG
1	D	1333	LEU

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Mol	Chain	Res	Type
1	D	1340	VAL
1	D	1341	GLU
1	D	1345	LEU
1	D	1346	THR
1	D	1347	LYS
1	D	1352	LEU
1	D	1355	SER
1	D	1363	ILE
1	D	1368	LYS
1	D	1372	LYS
1	D	1373	LYS
1	D	1387	ARG
1	D	1388	TYR
1	D	1389	LYS
1	D	1395	SER
1	D	1399	PHE
1	D	1403	MET
1	D	1407	VAL
1	D	1408	MET
1	D	1418	GLU
1	D	1436	ILE
1	D	1441	SER
1	D	1450	MET
1	D	1455	GLN
1	D	1457	LYS
1	D	1461	VAL
1	D	1463	SER
1	D	1466	LEU
1	D	1468	ARG
1	D	1470	LEU
1	D	1474	LYS
1	D	1483	LEU
1	D	1485	ILE
1	D	1529	ILE
1	D	1553	VAL
1	D	1577	MET
1	D	1579	LEU
1	D	1582	THR
1	D	1583	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1325	HIS
1	A	1332	GLN
1	A	1455	GLN
1	A	1472	HIS
1	B	1046	ASN
1	B	1332	GLN
1	B	1453	ASN
1	B	1538	GLN
1	C	1039	GLN
1	C	1046	ASN
1	C	1167	ASN
1	C	1210	ASN
1	C	1316	ASN
1	C	1552	ASN
1	C	1559	HIS
1	D	1039	GLN
1	D	1451	ASN

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	574/596 (96%)	-0.33	2 (0%) 90 78	60, 104, 157, 203	0
1	B	573/596 (96%)	-0.31	2 (0%) 90 78	65, 105, 187, 230	0
1	C	573/596 (96%)	-0.17	1 (0%) 91 81	60, 113, 212, 269	0
1	D	574/596 (96%)	-0.06	8 (1%) 73 52	68, 119, 215, 279	0
All	All	2294/2384 (96%)	-0.22	13 (0%) 85 69	60, 109, 199, 279	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1267	TYR	3.7
1	D	1274	VAL	3.1
1	D	1470	LEU	2.8
1	D	1269	LEU	2.7
1	B	1274	VAL	2.6
1	D	1271	ILE	2.5
1	C	1274	VAL	2.4
1	D	1264	TYR	2.4
1	D	1263	VAL	2.2
1	B	1470	LEU	2.1
1	D	1243	ILE	2.1
1	A	1577	MET	2.1
1	A	1472	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.