



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:20 AM UTC

PDB ID : 1XOI / pdb_00001xoi
Title : Human Liver Glycogen Phosphorylase A complexed with Chloroindoloyl glycine amide
Authors : Wright, S.W.; Rath, V.L.; Gibbs, E.M.; Treadway, J.L.
Deposited on : 2004-10-06
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

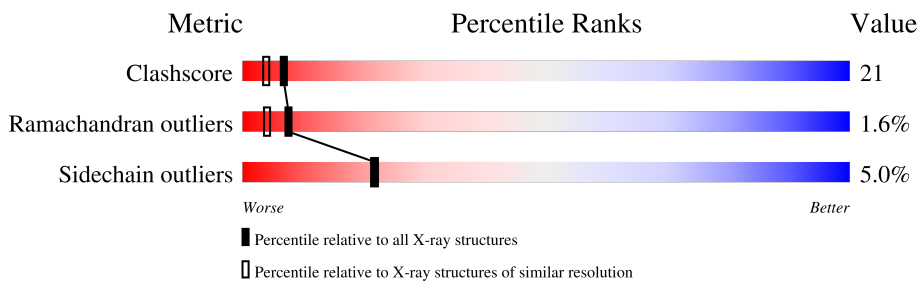
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	846	
1	B	846	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	288	A	862	X	-	-	-
4	288	B	1862	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13762 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.

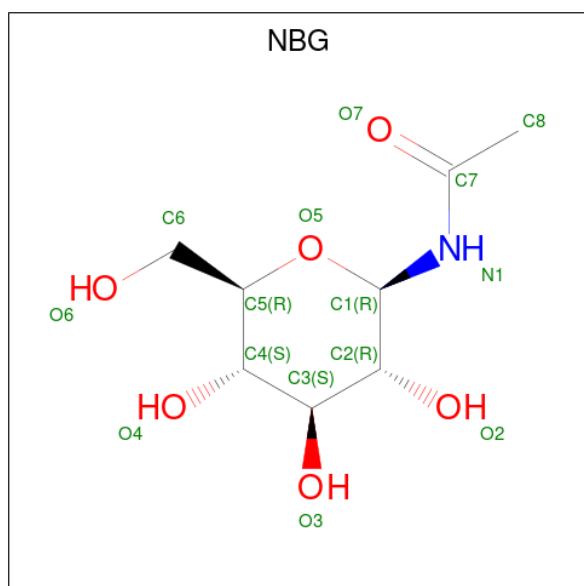
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			
1	B	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ALA	GLY	conflict	UNP P06737
B	1323	ALA	GLY	conflict	UNP P06737

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (CCD ID: NBG) (formula: $C_8H_{15}NO_6$).



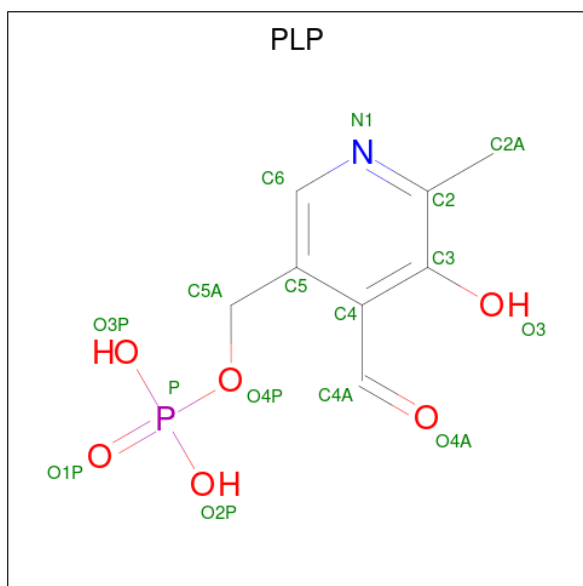
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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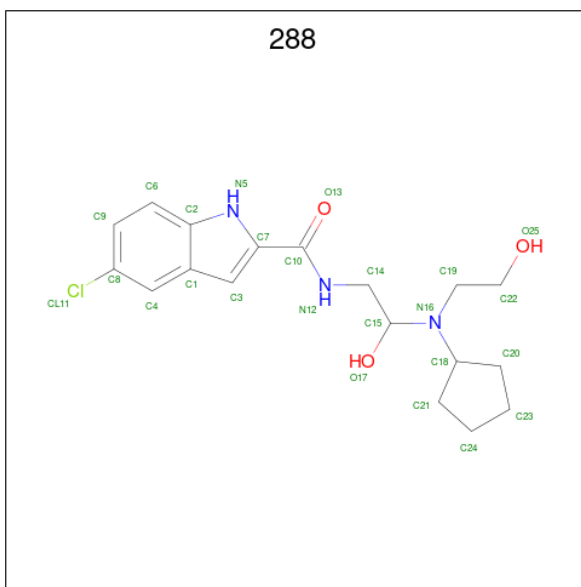
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is 5-CHLORO-1H-INDOLE-2-CARBOXYLIC ACID{[CYCLOPENTYL-(2-HYDROXY-ETHYL)-CARBAMOYL]-METHYL}-AMIDE (CCD ID: 288) (formula: $C_{18}H_{24}ClN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		
4	B	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		

- Molecule 5 is water.

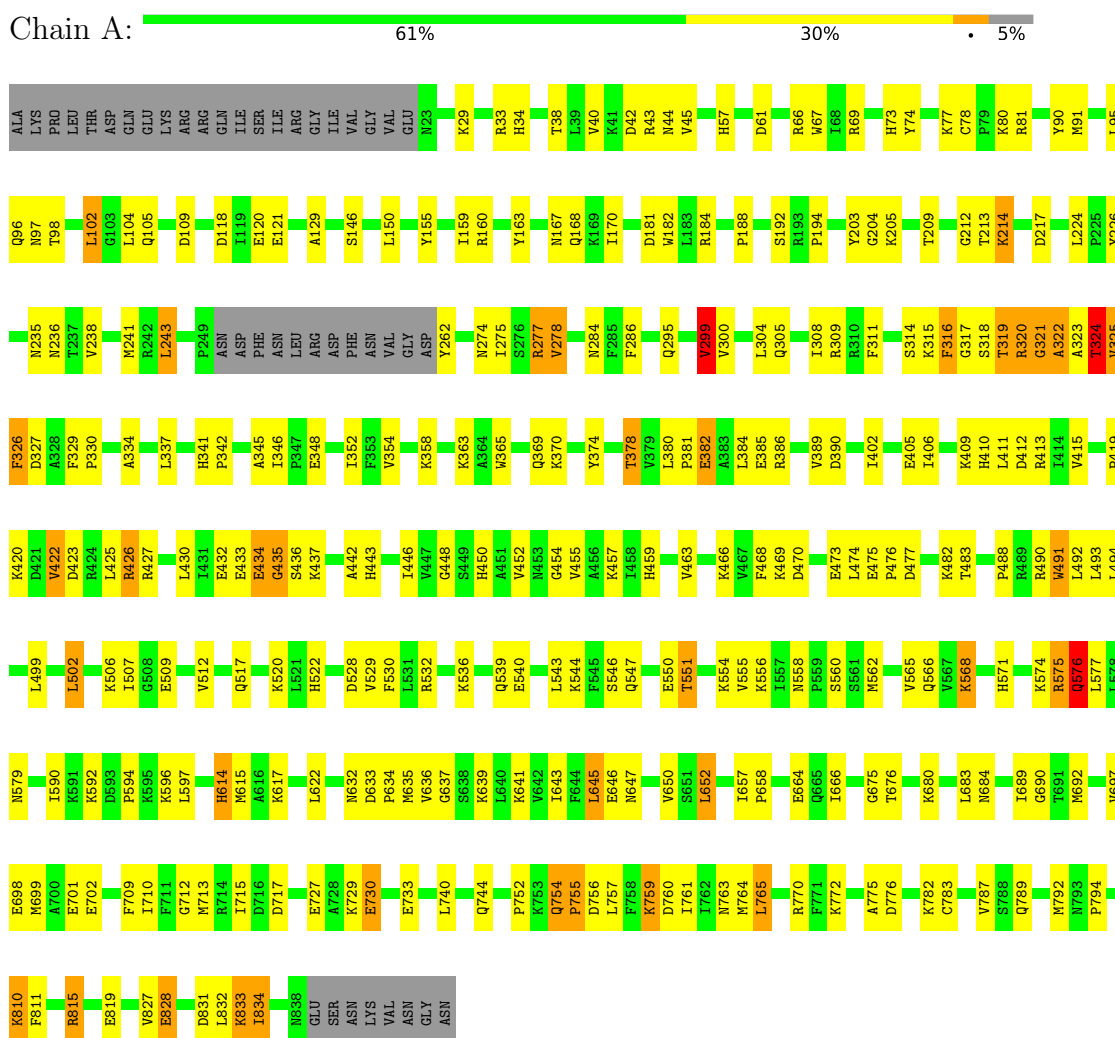
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	323	Total	O	0	0
			323	323		
5	B	313	Total	O	0	0
			313	313		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Glycogen phosphorylase, liver form



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E1828	F1711	G1607	K1506	P1419	A1323	I1216	L1095	ALA
P1829	G1712	K1608	I1507	K1420	T1324	L1224	Q1096	LYS
D1830	I1715	K1614	G1508	D1421	F1326	P1225	N1097	PRO
L1832	E1727	M1615	E1509	D1423	D1327	Y1226	T1098	THR
K1833	A1728	M1615	V1512	R1424	A1328	ASP	L1102	ASP
I1834	K1729	K1621	D1528	L1425	F1329	M1234	L1105	GLN
S1835	E1730	L1622	V1529	R1426	P1330	N1235	Q1105	GLU
L1836	E1733	M1632	F1530	L1427	A1334	N1236	T11237	GLY
S1837	E1734	D1633	L1531	L1430	A1337	V1238	A1111	ARG
N1838	A1734	P1634	R1532	I1431	L1243	W1244	I1112	ARG
GLU	P1736	M1635	K1536	E1433	H1341	P1342	Y1113	GLN
SER	V1636	V1636	Q1539	E1434	A1345	I1346	Q1114	TLE
ASN	K1639	K1640	E1540	G1435	I1347	P1347	G1116	ARG
VAL	L1640	L1641	L1543	K1437	E1348	ASP	L1117	GLY
ASN	Q1744	V1642	S1546	A1442	I1352	PHE	E1120	VAL
GLY	P1752	I1643	Q1547	H1443	F1353	ASN	E1121	GLY
ASN	K1753	F1644	Q1550	T1446	V1354	VAL	E1126	VAL
ASN	Q1754	L1645	T1551	V1447	W1365	GLY	E1127	VAL
ASN	P1755	E1646	K1552	G1448	Q1369	ASP	D1128	GLU
ASN	D1756	M1647	V1555	S1449	K1370	Y1262	L1150	E1026
ASN	L1757	F1758	K1556	H1450	T1371	R1269	L1155	L1027
	F1758	K1759	I1557	H1451	A1373	N1274	I1159	K1028
	K1759	S1651	V1558	N1452	F1372	I1275	R1160	K1029
	D1760	L1652	S1559	G1453	Y1374	S1276	I1163	R1033
	I1761	V1656	S1560	K1457	H1377	I1277	Y1166	H1034
	I1762	I1657	M1561	H1458	T1378	V1278	Q1167	T1038
	M1763	P1658	M1562	I1459	V1379	F1286	Q1168	L1039
	M1764	P1658	M1562	I1459	L1380	Q1295	Q1169	V1040
	L1765	I1666	M1562	I1459	P1381	Q1295	I1170	D1041
	R1770	I1666	M1562	I1459	E1382	Q1295	W1174	R1043
	F1771	S1674	V1565	I1462	E1385	V1299	D1181	V1044
	K1772	G1675	Q1566	V1463	R1386	V1300	D1182	V1045
	A1775	T1676	V1567	F1468	V1389	L1304	L1183	R1049
	D1776	G1677	K1568	D1470	D1390	L1304	R1184	D1061
	C1783	K1680	H1571	D1470	P1397	I1308	Y1185	Y1064
	K1786	L1683	K1574	E1473	I1402	K1312	S1192	W1067
	V1787	M1684	R1575	L1474	E1405	A1313	R1193	H1073
	Q1789	I1689	Q1576	E1475	I1406	K1314	P1194	Y1074
	M1792	G1690	L1578	P1476	K1409	F1316	Y1203	K1077
	M1793	T1691	N1579	D1477	K1409	G1317	V1206	C1078
	P1794	M1692	K1592	P1488	R1413	S1318	E1207	P1079
	L1802	V1697	D1593	V1491	I1415	T1319	H1208	K1080
	K1810	M1699	P1594	L1492	G1321	R1320	R1081	R1081
	D1814	E1701	K1596	L1493	V1415	A1322	N1210	M1091
	R1815	E1702	F1598	L1494				
	K1818	F1709	V1599	L1499				
		I1710	R1601	L1502				

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.91Å 123.91Å 123.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.6 (99.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13762	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 288, NBG, PLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/6653	0.93	24/8998 (0.3%)
1	B	0.42	0/6653	0.95	36/8998 (0.4%)
All	All	0.42	0/13306	0.94	60/17996 (0.3%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1565	VAL	N-CA-C	7.83	119.76	108.48
1	B	1754	GLN	CA-C-N	7.64	128.34	119.47
1	B	1754	GLN	C-N-CA	7.64	128.34	119.47
1	A	565	VAL	N-CA-C	7.62	119.46	108.48
1	A	754	GLN	CA-C-N	7.47	127.84	119.32
1	A	754	GLN	C-N-CA	7.47	127.84	119.32
1	B	1684	ASN	N-CA-C	7.34	121.09	112.72
1	B	1091	MET	N-CA-C	6.99	119.93	111.82
1	B	1064	VAL	N-CA-C	6.95	117.45	110.23
1	B	1380	LEU	CA-C-N	6.88	126.39	119.24
1	B	1380	LEU	C-N-CA	6.88	126.39	119.24
1	B	1323	ALA	N-CA-C	-6.87	96.46	108.20
1	A	91	MET	N-CA-C	6.83	120.84	112.23
1	A	507	ILE	N-CA-C	6.79	118.67	112.43
1	B	1105	GLN	N-CA-C	6.65	119.38	111.33
1	A	576	GLN	N-CA-C	-6.58	105.12	113.01
1	B	1576	GLN	N-CA-C	-6.49	105.23	113.01
1	B	1507	ILE	N-CA-C	6.48	118.39	112.43
1	B	1354	VAL	N-CA-C	6.45	116.61	110.74
1	A	684	ASN	N-CA-C	6.36	120.74	112.92
1	B	1650	VAL	N-CA-C	6.10	116.58	110.23
1	A	354	VAL	N-CA-C	6.07	116.26	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	VAL	CB-CA-C	-6.01	104.28	111.97
1	B	1299	VAL	CB-CA-C	-5.92	104.39	111.97
1	B	1699	MET	N-CA-C	-5.87	104.96	111.36
1	B	1831	ASP	N-CA-C	5.84	118.19	108.20
1	B	1193	ARG	CA-C-N	5.81	125.28	119.24
1	B	1193	ARG	C-N-CA	5.81	125.28	119.24
1	A	676	THR	N-CA-C	-5.72	108.10	114.62
1	B	1126	GLU	N-CA-C	5.69	118.58	110.10
1	A	454	GLY	N-CA-C	-5.62	103.70	112.58
1	A	378	THR	N-CA-C	5.62	118.89	109.95
1	A	699	MET	N-CA-C	-5.58	105.28	111.36
1	B	1454	GLY	N-CA-C	-5.57	103.78	112.58
1	A	675	GLY	N-CA-C	-5.54	105.77	112.48
1	A	203	TYR	CB-CA-C	-5.54	110.17	116.54
1	B	1676	THR	N-CA-C	-5.52	108.33	114.62
1	B	1633	ASP	CA-C-N	5.50	125.60	119.32
1	B	1633	ASP	C-N-CA	5.50	125.60	119.32
1	B	1314	SER	N-CA-C	5.46	118.75	112.97
1	B	1575	ARG	N-CA-C	5.36	119.03	111.52
1	A	614	HIS	N-CA-C	5.30	117.47	111.11
1	A	277	ARG	N-CA-C	5.30	116.86	111.14
1	A	182	TRP	N-CA-C	5.29	118.83	112.38
1	A	650	VAL	N-CA-C	5.28	115.72	110.23
1	A	129	ALA	N-CA-C	-5.28	99.38	108.56
1	B	1269	ARG	N-CA-C	-5.28	106.10	112.54
1	B	1203	TYR	CB-CA-C	-5.27	110.48	116.54
1	B	1182	TRP	N-CA-C	5.26	118.80	112.38
1	A	755	PRO	N-CA-C	5.25	121.57	113.75
1	B	1712	GLY	N-CA-C	5.21	121.76	112.22
1	B	1372	PHE	N-CA-C	5.16	118.52	110.32
1	B	1677	GLY	N-CA-C	-5.11	106.59	112.73
1	B	1216	ILE	N-CA-C	5.08	117.07	109.20
1	A	575	ARG	N-CA-C	5.07	118.62	111.52
1	B	1656	VAL	N-CA-C	5.07	115.84	110.72
1	B	1755	PRO	N-CA-C	5.06	121.15	113.81
1	A	491	TRP	N-CA-C	5.04	118.58	112.93
1	A	828	GLU	N-CA-C	5.02	118.21	107.91
1	B	1557	ILE	N-CA-C	5.01	115.79	108.58

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	6508	0	6518	293	0
1	B	6508	0	6518	274	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	1	0
3	B	15	0	7	0	0
4	A	25	0	22	0	0
4	B	25	0	22	3	0
5	A	323	0	0	52	0
5	B	313	0	0	33	0
All	All	13762	0	13124	561	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 21.

All (561) 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:1434:GLU:CD	1:B:1434:GLU:H	1.62	1.03
1:A:434:GLU:H	1:A:434:GLU:CD	1.65	1.01
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.10	0.98
1:A:236:ASN:HB3	1:A:834:ILE:HB	1.46	0.97
1:B:1168:GLN:HE21	1:B:1647:ASN:H	1.03	0.96
1:B:1170:ILE:HG12	1:B:1646:GLU:HG2	1.50	0.94
1:A:320:ARG:O	1:A:324:THR:HA	1.68	0.93
1:A:635:MET:HG2	5:A:1897:HOH:O	1.69	0.91
1:B:1049:ARG:HG2	1:B:1049:ARG:HH11	1.34	0.89
1:A:236:ASN:HD22	1:A:833:LYS:C	1.79	0.89
1:B:1592:LYS:O	1:B:1592:LYS:HD3	1.73	0.88
1:B:1323:ALA:C	1:B:1325:VAL:H	1.81	0.88
1:B:1029:LYS:HG2	1:B:1033:ARG:NH2	1.88	0.88
1:B:1236:ASN:HD22	1:B:1834:ILE:N	1.72	0.87
1:A:29:LYS:HG2	1:A:33:ARG:NH2	1.90	0.87
1:A:325:VAL:HG12	1:A:326:PHE:N	1.89	0.87
1:A:592:LYS:O	1:A:592:LYS:HD3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1831:ASP:C	1:B:1832:LEU:HD23	2.02	0.85
1:B:1168:GLN:NE2	1:B:1647:ASN:H	1.75	0.84
1:B:1692:MET:HG3	1:B:1697:VAL:HG22	1.60	0.83
1:B:1434:GLU:CD	1:B:1434:GLU:N	2.37	0.82
1:A:437:LYS:HD3	5:A:2292:HOH:O	1.79	0.81
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.61	0.81
1:B:1066:ARG:HD2	1:B:1236:ASN:HA	1.63	0.80
1:A:194:PRO:HD2	1:B:1049:ARG:HH21	1.46	0.80
1:A:763:ASN:HB3	5:A:2417:HOH:O	1.82	0.80
1:A:597:LEU:HG	5:A:2317:HOH:O	1.81	0.80
1:A:547:GLN:O	1:A:551:THR:HG23	1.80	0.79
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.63	0.79
1:A:434:GLU:CD	1:A:434:GLU:N	2.40	0.79
1:A:782:LYS:HD2	5:A:2090:HOH:O	1.84	0.78
1:B:1547:GLN:O	1:B:1551:THR:HG23	1.84	0.77
1:B:1023:ASN:HD21	1:B:1026:GLU:HG2	1.49	0.77
1:B:1236:ASN:HD22	1:B:1834:ILE:H	1.28	0.77
1:B:1315:LYS:HB3	5:B:2259:HOH:O	1.82	0.77
1:A:550:GLU:OE2	1:A:556:LYS:HD2	1.85	0.76
1:A:597:LEU:HB3	5:A:2434:HOH:O	1.82	0.76
1:B:1029:LYS:HE2	1:B:1033:ARG:NH2	2.00	0.76
1:A:380:LEU:HB3	1:A:382:GLU:OE2	1.85	0.76
1:A:29:LYS:HE2	1:A:33:ARG:NH2	2.00	0.76
1:A:433:GLU:HG3	1:A:437:LYS:HE3	1.68	0.76
1:B:1550:GLU:OE2	1:B:1556:LYS:HD2	1.85	0.76
1:B:1433:GLU:HG3	1:B:1437:LYS:HE3	1.68	0.76
1:A:325:VAL:C	1:A:327:ASP:H	1.94	0.75
1:A:96:GLN:NE2	1:A:105:GLN:HE22	1.84	0.75
1:B:1382:GLU:CD	1:B:1770:ARG:HH22	1.94	0.75
1:A:378:THR:HA	5:A:2036:HOH:O	1.87	0.74
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.67	0.74
1:B:1329:PHE:HB3	1:B:1330:PRO:HD3	1.68	0.74
1:A:236:ASN:HB2	1:A:834:ILE:H	1.53	0.73
1:B:1325:VAL:C	1:B:1327:ASP:H	1.97	0.73
1:A:262:TYR:N	5:A:1955:HOH:O	2.21	0.73
1:B:1170:ILE:HG12	1:B:1646:GLU:CG	2.19	0.73
1:B:1506:LYS:HE3	1:B:1530:PHE:HD1	1.53	0.72
1:A:120:GLU:HB2	5:A:2415:HOH:O	1.89	0.72
1:B:1096:GLN:HE21	1:B:1105:GLN:HE22	1.37	0.72
1:B:1405:GLU:OE2	1:B:1409:LYS:HE3	1.89	0.72
1:A:324:THR:O	1:A:325:VAL:HB	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:HD22	1:A:277:ARG:HD2	1.53	0.71
1:A:506:LYS:HE3	1:A:530:PHE:HD1	1.52	0.71
1:A:810:LYS:O	1:A:815:ARG:HD3	1.90	0.71
1:B:1274:ASN:HD22	1:B:1277:ARG:HD2	1.54	0.71
1:B:1810:LYS:O	1:B:1815:ARG:HD3	1.90	0.71
1:A:506:LYS:HE3	1:A:530:PHE:CD1	2.26	0.70
1:B:1159:ILE:HD11	1:B:1299:VAL:HG22	1.73	0.70
1:A:217:ASP:HB3	5:A:2270:HOH:O	1.90	0.70
1:B:1319:THR:CG2	1:B:1324:THR:HB	2.21	0.70
1:B:1455:VAL:H	1:B:1459:HIS:HD2	1.40	0.70
1:B:1322:ALA:HB3	5:B:2322:HOH:O	1.92	0.70
1:B:1262:TYR:N	5:B:1865:HOH:O	2.24	0.70
1:B:1763:ASN:HB3	5:B:2282:HOH:O	1.89	0.70
1:A:159:ILE:HD11	1:A:299:VAL:HG22	1.73	0.69
1:A:782:LYS:HB2	5:A:2090:HOH:O	1.93	0.69
1:B:1506:LYS:HE3	1:B:1530:PHE:CD1	2.28	0.69
1:A:236:ASN:ND2	1:A:833:LYS:HG3	2.07	0.69
1:B:1049:ARG:HH11	1:B:1049:ARG:CG	2.06	0.69
1:B:1437:LYS:HD3	5:B:2450:HOH:O	1.92	0.69
1:B:1550:GLU:HB2	5:B:2271:HOH:O	1.92	0.69
1:B:1323:ALA:C	1:B:1325:VAL:N	2.51	0.68
1:B:1772:LYS:HB3	1:B:1775:ALA:HB3	1.75	0.68
1:A:382:GLU:CD	1:A:770:ARG:HH22	2.02	0.68
1:A:405:GLU:OE2	1:A:409:LYS:HE3	1.94	0.68
1:A:96:GLN:HG2	1:A:494:LEU:HG	1.74	0.68
1:A:420:LYS:N	1:A:420:LYS:HD2	2.09	0.68
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.74	0.67
1:B:1509:GLU:O	1:B:1512:VAL:HG22	1.94	0.67
1:B:1770:ARG:HA	5:B:2478:HOH:O	1.94	0.67
1:A:455:VAL:H	1:A:459:HIS:HD2	1.40	0.67
1:A:118:ASP:OD1	1:A:121:GLU:HG3	1.94	0.67
1:B:1636:VAL:HG23	5:B:2210:HOH:O	1.94	0.67
1:A:316:PHE:HE1	1:A:325:VAL:HB	1.60	0.67
1:A:236:ASN:CB	1:A:834:ILE:H	2.08	0.67
1:A:571:HIS:H	1:A:576:GLN:NE2	1.92	0.67
1:A:509:GLU:O	1:A:512:VAL:HG22	1.95	0.66
1:B:1382:GLU:OE2	1:B:1770:ARG:NH2	2.27	0.66
1:B:1571:HIS:H	1:B:1576:GLN:NE2	1.93	0.66
1:B:1312:LYS:NZ	1:B:1326:PHE:HZ	1.93	0.66
1:A:308:ILE:HD13	1:A:352:ILE:HG21	1.78	0.65
1:A:319:THR:O	1:A:320:ARG:C	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.95	0.65
1:A:490:ARG:HD2	5:A:1877:HOH:O	1.96	0.65
1:B:1450:HIS:HD2	5:B:2088:HOH:O	1.79	0.64
1:A:309:ARG:HD3	5:A:2399:HOH:O	1.97	0.64
1:A:433:GLU:HA	1:A:437:LYS:HG2	1.80	0.64
1:B:1319:THR:HG23	1:B:1324:THR:HB	1.77	0.64
1:B:1433:GLU:HA	1:B:1437:LYS:HG2	1.80	0.64
1:B:1528:ASP:O	1:B:1532:ARG:HG3	1.98	0.64
1:B:1529:VAL:HA	1:B:1532:ARG:HD3	1.80	0.64
1:A:325:VAL:C	1:A:327:ASP:N	2.56	0.63
1:B:1174:TRP:CE2	1:B:1621:LYS:HG3	2.33	0.63
1:A:236:ASN:ND2	1:A:833:LYS:CG	2.61	0.63
1:B:1325:VAL:O	1:B:1327:ASP:N	2.30	0.63
1:A:29:LYS:HE2	1:A:33:ARG:HH21	1.64	0.63
1:A:319:THR:HA	5:A:2256:HOH:O	1.98	0.63
1:B:1320:ARG:HB3	5:B:2363:HOH:O	1.99	0.62
1:A:592:LYS:HD3	1:A:592:LYS:C	2.24	0.62
1:B:1274:ASN:ND2	1:B:1277:ARG:HH11	1.97	0.62
1:B:1562:MET:HE1	1:B:1787:VAL:HG12	1.81	0.62
1:B:1571:HIS:HB2	5:B:2345:HOH:O	1.99	0.62
1:B:1469:LYS:O	1:B:1473:GLU:HG3	2.00	0.62
1:B:1592:LYS:HD3	1:B:1592:LYS:C	2.23	0.62
1:A:633:ASP:O	1:A:636:VAL:HG22	1.99	0.62
1:A:286:PHE:CD1	1:A:385:GLU:HG2	2.34	0.62
1:B:1420:LYS:HD2	1:B:1420:LYS:N	2.15	0.62
1:B:1308:ILE:HD13	1:B:1352:ILE:HG21	1.82	0.61
1:A:236:ASN:HD22	1:A:834:ILE:N	1.98	0.61
1:A:562:MET:HE1	1:A:787:VAL:HG12	1.80	0.61
1:B:1633:ASP:O	1:B:1636:VAL:HG22	2.01	0.61
1:A:831:ASP:O	1:A:832:LEU:HD23	1.99	0.61
1:B:1536:LYS:O	1:B:1540:GLU:HG3	2.01	0.61
1:A:236:ASN:HD22	1:A:833:LYS:CA	2.13	0.61
1:A:325:VAL:CG1	1:A:326:PHE:N	2.61	0.61
1:B:1321:GLY:O	1:B:1323:ALA:C	2.43	0.61
1:B:1727:GLU:HG2	1:B:1729:LYS:HG2	1.82	0.61
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.84	0.60
1:B:1579:ASN:C	1:B:1579:ASN:HD22	2.10	0.60
1:B:1474:LEU:HD23	1:B:1474:LEU:O	2.01	0.60
1:A:529:VAL:HA	1:A:532:ARG:HD3	1.82	0.60
1:B:1234:MET:O	1:B:1833:LYS:HE3	2.02	0.60
1:A:536:LYS:O	1:A:540:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:O	1:A:744:GLN:HG3	2.01	0.60
1:A:168:GLN:HE21	1:A:647:ASN:H	1.50	0.60
1:A:756:ASP:HB3	5:A:2350:HOH:O	2.02	0.60
1:A:469:LYS:O	1:A:473:GLU:HG3	2.01	0.59
1:A:214:LYS:HD3	5:A:2316:HOH:O	2.03	0.59
1:B:1029:LYS:HE2	1:B:1033:ARG:HH21	1.65	0.59
1:B:1150:LEU:HB3	1:B:1829:PRO:HB3	1.84	0.59
1:A:380:LEU:HG	5:A:2357:HOH:O	2.01	0.59
1:A:474:LEU:HD23	1:A:474:LEU:O	2.02	0.59
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.85	0.59
1:A:109:ASP:HB3	5:A:1978:HOH:O	2.00	0.59
1:A:727:GLU:HG2	1:A:729:LYS:HG2	1.85	0.59
1:B:1170:ILE:CG1	1:B:1646:GLU:HG2	2.29	0.59
1:B:1286:PHE:CD1	1:B:1385:GLU:HG2	2.37	0.59
1:A:579:ASN:C	1:A:579:ASN:HD22	2.10	0.59
1:B:1325:VAL:C	1:B:1327:ASP:N	2.59	0.58
1:B:1023:ASN:HD21	1:B:1026:GLU:CG	2.15	0.58
1:B:1786:LYS:HD3	5:B:2411:HOH:O	2.03	0.58
1:A:522:HIS:NE2	5:A:2248:HOH:O	2.32	0.58
1:B:1160:ARG:HB2	1:B:1243:LEU:HB3	1.85	0.58
1:B:1314:SER:O	1:B:1315:LYS:C	2.45	0.58
1:B:1023:ASN:N	5:B:2431:HOH:O	2.36	0.58
1:B:1034:HIS:HD2	1:B:1038:THR:OG1	1.87	0.58
1:B:1709:PHE:HB3	1:B:1783:CYS:SG	2.44	0.58
1:B:1034:HIS:HE1	1:B:1061:ASP:OD2	1.85	0.58
1:A:554:LYS:HA	5:A:2336:HOH:O	2.03	0.58
1:B:1323:ALA:O	1:B:1325:VAL:N	2.36	0.58
1:B:1733:GLU:HB2	5:B:2281:HOH:O	2.02	0.58
1:B:1740:LEU:O	1:B:1744:GLN:HG3	2.04	0.58
1:A:236:ASN:CB	1:A:834:ILE:N	2.67	0.57
1:B:1274:ASN:ND2	1:B:1277:ARG:HD2	2.19	0.57
1:B:1599:VAL:HB	5:B:2413:HOH:O	2.02	0.57
1:B:1639:LYS:NZ	5:B:2324:HOH:O	2.37	0.57
1:B:1170:ILE:HB	1:B:1646:GLU:OE2	2.05	0.57
1:A:536:LYS:O	1:A:539:GLN:HB3	2.04	0.57
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.45	0.57
1:B:1049:ARG:NH2	5:B:2228:HOH:O	2.37	0.57
1:A:66:ARG:CD	1:A:236:ASN:HA	2.35	0.57
1:A:325:VAL:O	1:A:327:ASP:N	2.38	0.57
1:A:422:VAL:HG23	1:A:423:ASP:N	2.19	0.57
1:A:327:ASP:OD1	1:A:363:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:HB3	1:A:834:ILE:CB	2.29	0.56
1:A:697:VAL:O	1:A:701:GLU:HG3	2.06	0.56
1:B:1111:ALA:O	1:B:1115:LEU:HG	2.05	0.56
1:B:1316:PHE:O	1:B:1318:SER:N	2.38	0.56
1:B:1536:LYS:O	1:B:1539:GLN:HB3	2.04	0.56
1:B:1066:ARG:CD	1:B:1236:ASN:HA	2.35	0.56
1:B:1433:GLU:CG	1:B:1437:LYS:HE3	2.35	0.56
1:A:422:VAL:CG2	1:A:423:ASP:N	2.68	0.56
1:B:1419:PRO:HB2	1:B:1420:LYS:HD2	1.88	0.56
1:B:1321:GLY:O	1:B:1323:ALA:N	2.38	0.56
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.86	0.56
1:A:274:ASN:ND2	1:A:277:ARG:HD2	2.20	0.56
1:A:433:GLU:CG	1:A:437:LYS:HE3	2.35	0.56
1:A:532:ARG:NE	5:A:2037:HOH:O	2.37	0.56
1:B:1571:HIS:H	1:B:1576:GLN:HE22	1.53	0.56
1:A:575:ARG:HH22	1:A:776:ASP:HB2	1.70	0.56
1:B:1422:VAL:HG23	1:B:1423:ASP:N	2.21	0.56
1:B:1433:GLU:O	1:B:1434:GLU:C	2.49	0.56
1:B:1697:VAL:O	1:B:1701:GLU:HG3	2.06	0.56
1:A:73:HIS:CE1	1:A:77:LYS:HG3	2.41	0.56
1:A:325:VAL:HG12	1:A:326:PHE:H	1.69	0.56
1:A:474:LEU:HD22	1:A:475:GLU:HG3	1.88	0.55
1:A:571:HIS:H	1:A:576:GLN:HE22	1.52	0.55
1:B:1474:LEU:HD22	1:B:1475:GLU:HG3	1.88	0.55
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.35	0.55
1:A:319:THR:O	1:A:320:ARG:O	2.24	0.55
1:B:1413:ARG:HA	1:B:1413:ARG:NE	2.22	0.55
1:B:1236:ASN:ND2	1:B:1834:ILE:N	2.51	0.55
1:A:69:ARG:HB2	1:A:834:ILE:HD13	1.88	0.55
1:B:1207:GLU:HG2	1:B:1209:THR:HG23	1.88	0.55
1:B:1207:GLU:HG2	1:B:1209:THR:CG2	2.36	0.55
1:B:1422:VAL:CG2	1:B:1423:ASP:N	2.70	0.55
1:B:1450:HIS:HE1	5:B:2026:HOH:O	1.89	0.55
1:B:1575:ARG:HH22	1:B:1776:ASP:HB2	1.72	0.55
1:A:528:ASP:O	1:A:532:ARG:HG3	2.06	0.55
1:B:1312:LYS:HZ2	1:B:1326:PHE:HZ	1.54	0.55
1:B:1308:ILE:CD1	1:B:1352:ILE:HG21	2.37	0.55
1:A:284:ASN:ND2	5:A:2036:HOH:O	2.40	0.55
1:A:419:PRO:HB2	1:A:420:LYS:HD2	1.87	0.54
1:B:1325:VAL:HG12	1:B:1327:ASP:HB2	1.89	0.54
1:A:66:ARG:HG2	1:A:834:ILE:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:O	1:A:317:GLY:C	2.48	0.54
1:B:1834:ILE:O	1:B:1835:SER:C	2.49	0.54
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.90	0.54
1:A:433:GLU:O	1:A:434:GLU:C	2.49	0.54
1:A:98:THR:HG22	1:A:102:LEU:HD22	1.88	0.54
1:B:1029:LYS:HG2	1:B:1033:ARG:HH22	1.70	0.54
1:A:194:PRO:CD	1:B:1049:ARG:HH21	2.18	0.54
1:A:275:ILE:O	1:A:295:GLN:HG2	2.08	0.54
1:A:96:GLN:HE21	1:A:105:GLN:NE2	1.92	0.54
1:B:1325:VAL:HB	5:B:2234:HOH:O	2.07	0.54
1:B:1457:LYS:HE2	1:B:1698:GLU:HG2	1.88	0.54
1:A:214:LYS:HB3	1:A:214:LYS:HZ2	1.73	0.54
1:B:1377:HIS:O	1:B:1378:THR:HB	2.08	0.54
1:B:1551:THR:HG22	5:B:2271:HOH:O	2.07	0.54
1:A:120:GLU:OE2	1:A:544:LYS:NZ	2.27	0.53
1:A:413:ARG:HA	1:A:413:ARG:NE	2.24	0.53
1:B:1409:LYS:NZ	5:B:2361:HOH:O	2.34	0.53
1:A:236:ASN:O	1:A:834:ILE:HD12	2.09	0.53
1:B:1023:ASN:ND2	1:B:1026:GLU:H	2.05	0.53
1:B:1754:GLN:NE2	1:B:1757:LEU:HD13	2.22	0.53
1:B:1320:ARG:NH1	5:B:2014:HOH:O	2.40	0.53
1:B:1434:GLU:O	1:B:1435:GLY:C	2.52	0.53
1:B:1657:ILE:HB	1:B:1658:PRO:HD3	1.90	0.53
1:B:1275:ILE:O	1:B:1295:GLN:HG2	2.07	0.53
1:A:74:TYR:HB3	1:A:81:ARG:HH12	1.74	0.53
1:A:212:GLY:HA3	1:A:358:LYS:NZ	2.24	0.53
1:A:575:ARG:HD3	1:A:666:ILE:O	2.09	0.53
1:A:754:GLN:NE2	1:A:757:LEU:HD13	2.24	0.52
1:B:1379:VAL:HG12	1:B:1379:VAL:O	2.08	0.52
1:A:597:LEU:HD22	5:A:2434:HOH:O	2.08	0.52
1:B:1170:ILE:CG1	1:B:1646:GLU:CG	2.86	0.52
1:B:1174:TRP:CZ2	1:B:1621:LYS:HG3	2.44	0.52
1:B:1365:TRP:CD1	1:B:1369:GLN:NE2	2.78	0.52
1:A:423:ASP:OD2	1:A:426:ARG:NH1	2.43	0.52
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.92	0.52
1:B:1098:THR:O	1:B:1102:LEU:HD13	2.09	0.52
1:B:1300:VAL:HG13	1:B:1345:ALA:HA	1.91	0.52
1:B:1831:ASP:O	1:B:1832:LEU:HD23	2.09	0.52
1:A:194:PRO:HG2	1:B:1049:ARG:HE	1.74	0.52
1:A:57:HIS:HE1	4:B:1862:288:H202	1.73	0.51
1:B:1488:PRO:O	1:B:1492:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:TYR:HB3	1:B:1081:ARG:HH12	1.76	0.51
1:B:1756:ASP:HB2	1:B:1759:LYS:HZ3	1.76	0.51
1:A:756:ASP:HB2	1:A:759:LYS:HZ3	1.76	0.51
1:B:1073:HIS:CE1	1:B:1077:LYS:HG3	2.46	0.51
1:B:1555:VAL:HG21	1:B:1643:ILE:HD11	1.93	0.51
1:B:1067:TRP:HA	1:B:1238:VAL:HB	1.93	0.51
1:B:1096:GLN:HG2	1:B:1494:LEU:HG	1.93	0.51
1:B:1168:GLN:HE21	1:B:1647:ASN:N	1.87	0.51
1:A:488:PRO:O	1:A:492:LEU:HB3	2.10	0.51
1:B:1415:VAL:HG23	1:B:1425:LEU:HD21	1.93	0.51
1:A:67:TRP:HA	1:A:238:VAL:HB	1.93	0.51
1:B:1192:SER:C	1:B:1194:PRO:HD3	2.36	0.51
1:B:1224:LEU:HG	1:B:1226:TYR:CE2	2.46	0.50
1:A:632:ASN:O	1:A:634:PRO:HD3	2.12	0.50
1:A:764:MET:C	1:A:764:MET:SD	2.94	0.50
1:A:321:GLY:HA2	5:A:2388:HOH:O	2.11	0.50
1:A:410:HIS:HD2	5:A:2377:HOH:O	1.93	0.50
1:A:224:LEU:HG	1:A:226:TYR:CE2	2.47	0.50
1:B:1601:ARG:NE	5:B:2296:HOH:O	2.44	0.50
1:A:506:LYS:HE2	5:A:2309:HOH:O	2.10	0.50
1:B:1028:LYS:HD3	1:B:1114:GLN:HB2	1.93	0.50
1:B:1615:MET:HE1	1:B:1761:ILE:HG12	1.93	0.50
1:B:1575:ARG:HD3	1:B:1666:ILE:O	2.11	0.50
1:A:305:GLN:HG2	5:A:2485:HOH:O	2.12	0.49
1:A:365:TRP:CD1	1:A:369:GLN:NE2	2.79	0.49
1:B:1206:VAL:HG23	1:B:1397:PRO:HB2	1.92	0.49
1:B:1326:PHE:N	5:B:2234:HOH:O	2.45	0.49
1:A:315:LYS:O	1:A:316:PHE:O	2.30	0.49
1:B:1049:ARG:HD3	5:B:1962:HOH:O	2.11	0.49
1:B:1346:ILE:HD13	1:B:1448:GLY:HA3	1.93	0.49
1:A:702:GLU:HG3	1:A:810:LYS:HG2	1.93	0.49
1:A:192:SER:C	1:A:194:PRO:HD3	2.38	0.49
1:A:236:ASN:HB2	1:A:834:ILE:N	2.24	0.49
1:A:423:ASP:HA	1:A:426:ARG:NE	2.28	0.49
1:A:555:VAL:HG21	1:A:643:ILE:HD11	1.95	0.49
1:A:194:PRO:HG2	1:B:1049:ARG:NE	2.27	0.49
1:A:466:LYS:NZ	5:A:2441:HOH:O	2.44	0.49
1:A:772:LYS:N	1:A:772:LYS:HD2	2.28	0.49
1:B:1574:LYS:HB2	1:B:1576:GLN:HE22	1.77	0.49
1:B:1689:ILE:HG23	1:B:1689:ILE:O	2.12	0.49
1:B:1121:GLU:HB2	5:B:2442:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HG23	1:A:425:LEU:HD21	1.94	0.49
1:A:575:ARG:NH2	1:A:776:ASP:HB2	2.28	0.49
1:A:733:GLU:HG3	1:A:733:GLU:O	2.13	0.49
1:B:1185:TYR:HB2	5:B:2269:HOH:O	2.13	0.49
1:B:1325:VAL:HG12	1:B:1327:ASP:CB	2.43	0.49
1:B:1423:ASP:HA	1:B:1426:ARG:NE	2.28	0.49
1:B:1756:ASP:HB2	1:B:1759:LYS:NZ	2.27	0.49
1:A:434:GLU:O	1:A:435:GLY:C	2.55	0.49
1:B:1435:GLY:O	1:B:1436:SER:C	2.54	0.49
1:A:756:ASP:HB2	1:A:759:LYS:NZ	2.28	0.48
1:A:789:GLN:HG3	5:A:2353:HOH:O	2.12	0.48
1:A:492:LEU:C	1:A:492:LEU:HD13	2.38	0.48
1:A:689:ILE:HG23	1:A:689:ILE:O	2.13	0.48
1:A:435:GLY:O	1:A:436:SER:C	2.56	0.48
1:A:492:LEU:CD1	1:A:493:LEU:HD23	2.44	0.48
1:A:690:GLY:O	1:A:710:ILE:HA	2.12	0.48
1:A:304:LEU:HD12	1:A:348:GLU:CG	2.44	0.48
1:B:1312:LYS:HE3	1:B:1324:THR:HG21	1.95	0.48
1:A:205:LYS:NZ	1:A:217:ASP:OD2	2.41	0.48
1:A:434:GLU:N	1:A:434:GLU:OE1	2.47	0.48
1:B:1462:ILE:HD11	1:B:1715:ILE:HD12	1.96	0.48
1:B:1575:ARG:NH2	1:B:1776:ASP:HB2	2.29	0.48
1:B:1772:LYS:HD2	1:B:1772:LYS:N	2.28	0.48
1:A:494:LEU:HD23	1:A:494:LEU:C	2.39	0.48
1:A:450:HIS:HD2	5:A:2209:HOH:O	1.96	0.48
1:B:1181:ASP:OD2	1:B:1184:ARG:NE	2.47	0.48
1:A:381:PRO:HD2	1:A:382:GLU:OE2	2.13	0.47
1:A:474:LEU:HD23	1:A:474:LEU:C	2.39	0.47
1:B:1462:ILE:HD11	1:B:1715:ILE:CD1	2.44	0.47
1:B:1492:LEU:HD13	1:B:1492:LEU:C	2.39	0.47
1:A:43:ARG:HD3	5:A:1984:HOH:O	2.15	0.47
1:A:491:TRP:CZ2	1:A:680:LYS:NZ	2.77	0.47
1:A:324:THR:O	1:A:324:THR:OG1	2.31	0.47
1:B:1236:ASN:ND2	1:B:1833:LYS:HB3	2.29	0.47
1:B:1423:ASP:OD2	1:B:1426:ARG:NH1	2.47	0.47
1:B:1632:ASN:O	1:B:1634:PRO:HD3	2.13	0.47
1:B:1702:GLU:HG3	1:B:1810:LYS:HG2	1.95	0.47
1:A:419:PRO:HB2	1:A:420:LYS:NZ	2.29	0.47
1:B:1546:SER:O	1:B:1550:GLU:HG3	2.15	0.47
1:B:1764:MET:SD	1:B:1764:MET:C	2.97	0.47
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:NH2	1:A:432:GLU:OE1	2.44	0.47
1:B:1690:GLY:O	1:B:1710:ILE:HA	2.13	0.47
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.96	0.47
1:B:1168:GLN:NE2	1:B:1647:ASN:N	2.54	0.47
1:B:1568:LYS:HD3	1:B:1574:LYS:HD2	1.97	0.47
1:B:1596:LYS:HG2	1:B:1597:LEU:N	2.28	0.47
1:A:319:THR:HG23	5:A:2256:HOH:O	2.14	0.47
1:A:305:GLN:HB2	5:A:2279:HOH:O	2.14	0.47
1:A:319:THR:CA	5:A:2256:HOH:O	2.60	0.47
1:B:1321:GLY:O	1:B:1322:ALA:C	2.57	0.47
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.48	0.46
1:A:546:SER:O	1:A:550:GLU:HG3	2.14	0.46
1:B:1474:LEU:HD23	1:B:1474:LEU:C	2.38	0.46
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.45	0.46
1:A:316:PHE:CE2	1:A:319:THR:HG22	2.49	0.46
1:A:370:LYS:HD2	5:A:2457:HOH:O	2.15	0.46
1:A:378:THR:HG21	1:A:384:LEU:HD23	1.96	0.46
1:A:457:LYS:HE2	1:A:698:GLU:HG2	1.96	0.46
1:A:118:ASP:CG	1:A:121:GLU:HG3	2.40	0.46
1:B:1555:VAL:HG21	1:B:1643:ILE:CD1	2.46	0.46
1:A:322:ALA:O	1:A:324:THR:HG23	2.16	0.46
1:A:792:MET:O	1:A:794:PRO:HD3	2.15	0.46
1:B:1224:LEU:HD21	5:B:1977:HOH:O	2.16	0.46
1:B:1325:VAL:HG12	1:B:1327:ASP:CG	2.40	0.46
1:A:44:ASN:OD1	1:A:45:VAL:HG23	2.15	0.46
1:A:574:LYS:HB2	1:A:576:GLN:HE22	1.80	0.46
1:B:1096:GLN:NE2	1:B:1105:GLN:HE22	2.11	0.46
1:B:1492:LEU:CD1	1:B:1493:LEU:HD23	2.46	0.46
1:A:833:LYS:HG3	1:A:833:LYS:O	2.15	0.46
1:B:1434:GLU:N	1:B:1434:GLU:OE1	2.48	0.46
1:B:1733:GLU:O	1:B:1733:GLU:HG3	2.15	0.46
1:A:558:ASN:OD1	1:A:560:SER:HB3	2.16	0.46
1:A:74:TYR:HB3	1:A:81:ARG:NH1	2.31	0.46
1:A:205:LYS:HA	5:A:2480:HOH:O	2.15	0.46
1:A:97:ASN:HA	1:A:494:LEU:HD12	1.98	0.45
1:A:330:PRO:HB2	1:A:370:LYS:HZ2	1.81	0.45
1:A:405:GLU:HA	5:A:2300:HOH:O	2.15	0.45
1:B:1314:SER:O	1:B:1315:LYS:O	2.33	0.45
1:B:1419:PRO:HB2	1:B:1420:LYS:NZ	2.30	0.45
1:B:1752:PRO:HB2	1:B:1753:LYS:HZ2	1.81	0.45
1:A:109:ASP:CB	5:A:1978:HOH:O	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.97	0.45
1:A:320:ARG:O	1:A:324:THR:CA	2.54	0.45
1:B:1316:PHE:O	1:B:1317:GLY:C	2.58	0.45
1:B:1547:GLN:NE2	5:B:2366:HOH:O	2.48	0.45
1:A:188:PRO:HB3	4:B:1862:288:H232	1.98	0.45
1:A:772:LYS:HE2	5:A:2137:HOH:O	2.15	0.45
1:B:1455:VAL:HG23	1:B:1674:SER:HB2	1.99	0.45
1:B:1494:LEU:C	1:B:1494:LEU:HD23	2.41	0.45
1:A:636:VAL:O	1:A:639:LYS:HG3	2.17	0.45
1:B:1304:LEU:HD12	1:B:1348:GLU:CG	2.46	0.45
1:B:1832:LEU:O	1:B:1833:LYS:HG3	2.17	0.45
1:A:236:ASN:ND2	1:A:834:ILE:N	2.64	0.45
1:A:502:LEU:HD22	1:A:530:PHE:HE1	1.82	0.45
1:A:596:LYS:HG2	1:A:597:LEU:N	2.30	0.45
1:B:1300:VAL:CG1	1:B:1345:ALA:HA	2.47	0.45
1:B:1319:THR:O	1:B:1320:ARG:C	2.60	0.45
1:A:146:SER:O	1:A:150:LEU:HD13	2.16	0.45
1:A:555:VAL:HG21	1:A:643:ILE:CD1	2.47	0.45
1:B:1080:LYS:HE2	1:B:1334:ALA:HB2	1.99	0.45
1:A:463:VAL:HG13	1:A:468:PHE:CD1	2.52	0.45
1:A:544:LYS:HD3	5:A:2335:HOH:O	2.16	0.45
1:A:712:GLY:HA2	5:A:2075:HOH:O	2.17	0.45
1:B:1044:ASN:OD1	1:B:1045:VAL:HG23	2.17	0.45
1:A:492:LEU:HD13	1:A:493:LEU:N	2.31	0.45
1:A:727:GLU:O	1:A:730:GLU:HB2	2.17	0.45
1:B:1074:TYR:HB3	1:B:1081:ARG:NH1	2.32	0.45
1:B:1081:ARG:NH1	1:B:1155:TYR:OH	2.50	0.45
1:A:236:ASN:HD22	1:A:833:LYS:HG3	1.82	0.44
1:A:316:PHE:N	1:A:316:PHE:CD2	2.85	0.44
1:A:789:GLN:HA	1:A:792:MET:HE3	1.99	0.44
1:B:1023:ASN:C	1:B:1023:ASN:HD22	2.24	0.44
1:B:1502:LEU:HD22	1:B:1530:PHE:HE1	1.82	0.44
1:B:1727:GLU:O	1:B:1730:GLU:HB2	2.17	0.44
1:A:236:ASN:HD21	1:A:833:LYS:HG3	1.78	0.44
1:A:315:LYS:O	1:A:316:PHE:C	2.59	0.44
1:A:96:GLN:NE2	1:A:105:GLN:NE2	2.60	0.44
1:B:1530:PHE:HE2	1:B:1802:LEU:HD13	1.82	0.44
1:A:236:ASN:HD21	1:A:833:LYS:CG	2.28	0.44
1:A:483:THR:O	1:A:815:ARG:NH2	2.44	0.44
1:B:1571:HIS:O	1:B:1576:GLN:NE2	2.50	0.44
1:B:1614:HIS:HE1	1:B:1760:ASP:OD1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD12	1:A:348:GLU:HG3	1.99	0.44
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.51	0.44
1:A:323:ALA:HB1	5:A:2238:HOH:O	2.18	0.44
1:B:1023:ASN:ND2	1:B:1023:ASN:C	2.72	0.44
1:A:274:ASN:HA	1:A:277:ARG:HB2	2.00	0.43
1:A:566:GLN:HA	5:A:2143:HOH:O	2.18	0.43
1:B:1023:ASN:N	1:B:1023:ASN:HD22	2.15	0.43
1:B:1575:ARG:C	1:B:1577:LEU:N	2.73	0.43
1:A:772:LYS:HD3	5:A:2380:HOH:O	2.18	0.43
1:B:1235:ASN:O	1:B:1236:ASN:HB2	2.18	0.43
1:B:1430:LEU:CD2	1:B:1443:HIS:HB3	2.48	0.43
1:B:1442:ALA:O	1:B:1446:ILE:HG13	2.18	0.43
1:B:1492:LEU:HD13	1:B:1493:LEU:N	2.32	0.43
1:A:236:ASN:HD21	1:A:833:LYS:CD	2.31	0.43
1:B:1374:TYR:O	1:B:1452:VAL:HA	2.18	0.43
1:B:1759:LYS:NZ	1:B:1759:LYS:HB2	2.33	0.43
1:A:554:LYS:HD2	5:A:2346:HOH:O	2.17	0.43
1:A:568:LYS:HD3	1:A:574:LYS:HD2	1.99	0.43
1:B:1166:PHE:O	1:B:1608:LYS:NZ	2.51	0.43
1:A:517:GLN:OE1	1:A:520:LYS:HE3	2.19	0.43
1:B:1832:LEU:C	1:B:1833:LYS:HG3	2.44	0.43
1:A:590:ILE:HG21	1:A:636:VAL:HG12	2.01	0.43
1:A:729:LYS:O	1:A:730:GLU:C	2.62	0.43
1:B:1427:ARG:HH21	1:B:1470:ASP:CG	2.26	0.43
1:A:614:HIS:HE1	1:A:760:ASP:OD1	2.02	0.43
1:B:1402:ILE:O	1:B:1406:ILE:HG13	2.19	0.43
1:B:1789:GLN:HA	1:B:1792:MET:HE3	2.01	0.43
1:A:236:ASN:HD21	1:A:833:LYS:HD2	1.84	0.43
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.64	0.43
1:A:311:PHE:O	1:A:314:SER:OG	2.33	0.43
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.83	0.43
1:A:727:GLU:OE2	1:A:730:GLU:OE2	2.36	0.43
1:A:402:ILE:O	1:A:406:ILE:HG13	2.18	0.43
1:B:1128:ASP:OD2	1:B:1651:SER:HB3	2.18	0.43
1:B:1641:LYS:HA	1:B:1641:LYS:HD3	1.76	0.43
1:B:1752:PRO:O	1:B:1755:PRO:HD3	2.19	0.43
1:A:389:VAL:HG23	1:A:390:ASP:N	2.34	0.42
1:A:430:LEU:CD2	1:A:443:HIS:HB3	2.49	0.42
1:A:571:HIS:HB3	1:A:574:LYS:HG2	2.00	0.42
1:A:29:LYS:HG2	1:A:33:ARG:HH22	1.74	0.42
1:B:1023:ASN:ND2	1:B:1023:ASN:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:ASP:OD2	1:B:1042:ASP:C	2.62	0.42
1:B:1463:VAL:HG13	1:B:1468:PHE:CD1	2.53	0.42
1:B:1571:HIS:HB3	1:B:1574:LYS:HG2	2.01	0.42
1:A:544:LYS:NZ	5:A:2335:HOH:O	2.51	0.42
1:A:566:GLN:HB2	1:A:664:GLU:HB2	2.02	0.42
1:B:1735:LEU:HA	1:B:1736:PRO:HD2	1.91	0.42
1:A:42:ASP:OD2	1:A:42:ASP:C	2.62	0.42
1:A:235:ASN:O	1:A:236:ASN:HB2	2.19	0.42
1:A:374:TYR:O	1:A:452:VAL:HA	2.20	0.42
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.90	0.42
1:B:1491:TRP:CZ2	1:B:1680:LYS:NZ	2.77	0.42
1:B:1555:VAL:HG12	1:B:1556:LYS:N	2.34	0.42
1:B:1792:MET:O	1:B:1794:PRO:HD3	2.19	0.42
1:A:633:ASP:OD2	1:A:633:ASP:C	2.62	0.42
1:B:1225:PRO:HD3	1:B:1244:TRP:CZ3	2.54	0.42
1:B:1601:ARG:CZ	5:B:2296:HOH:O	2.67	0.42
1:B:1831:ASP:O	1:B:1831:ASP:CG	2.62	0.42
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.01	0.42
1:B:1636:VAL:O	1:B:1639:LYS:HG3	2.20	0.42
1:A:411:LEU:O	1:A:412:ASP:C	2.63	0.42
1:A:636:VAL:HG23	1:A:637:GLY:N	2.34	0.42
1:B:1304:LEU:HD12	1:B:1348:GLU:HG3	2.01	0.42
1:A:57:HIS:CE1	4:B:1862:288:H202	2.54	0.42
1:A:450:HIS:HE1	5:A:2305:HOH:O	2.02	0.42
1:A:482:LYS:HE3	1:A:819:GLU:C	2.44	0.42
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.88	0.42
1:A:759:LYS:NZ	1:A:759:LYS:HB2	2.34	0.42
1:B:1566:GLN:HE22	1:B:1576:GLN:HA	1.84	0.42
1:B:1754:GLN:N	1:B:1755:PRO:HD3	2.34	0.42
1:A:45:VAL:O	1:A:45:VAL:HG12	2.20	0.42
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.02	0.42
1:A:752:PRO:C	1:A:754:GLN:H	2.28	0.42
1:A:420:LYS:HD2	1:A:420:LYS:H	1.84	0.42
1:B:1579:ASN:C	1:B:1579:ASN:ND2	2.77	0.42
1:A:80:LYS:HB3	1:A:827:VAL:HG12	2.02	0.41
1:A:163:TYR:HB2	1:A:278:VAL:HG13	2.01	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.35	0.41
1:B:1330:PRO:HB2	1:B:1370:LYS:HZ2	1.84	0.41
1:B:1543:LEU:HD12	1:B:1543:LEU:HA	1.87	0.41
1:A:641:LYS:HD3	1:A:641:LYS:HA	1.78	0.41
1:B:1163:TYR:HB2	1:B:1278:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1210:ASN:H	1:B:1210:ASN:ND2	2.18	0.41
1:A:442:ALA:O	1:A:446:ILE:HG13	2.19	0.41
1:A:532:ARG:CZ	5:A:2037:HOH:O	2.68	0.41
1:A:571:HIS:O	1:A:576:GLN:NE2	2.54	0.41
1:A:645:LEU:HD13	1:A:652:LEU:HD13	2.02	0.41
1:B:1389:VAL:HG23	1:B:1390:ASP:N	2.35	0.41
1:B:1415:VAL:CG2	1:B:1425:LEU:HD11	2.50	0.41
1:B:1814:ASP:O	1:B:1818:LYS:HG3	2.20	0.41
1:B:1341:HIS:HB2	1:B:1342:PRO:HD3	2.02	0.41
1:B:1727:GLU:OE2	1:B:1730:GLU:OE2	2.38	0.41
1:A:236:ASN:ND2	1:A:833:LYS:CB	2.84	0.41
1:A:330:PRO:CB	1:A:370:LYS:HZ2	2.33	0.41
1:A:617:LYS:HD3	5:A:1895:HOH:O	2.21	0.41
1:A:834:ILE:O	1:A:834:ILE:HG22	2.21	0.41
1:B:1112:ILE:HG23	1:B:1117:LEU:HB2	2.01	0.41
1:B:1170:ILE:HG12	1:B:1646:GLU:CD	2.46	0.41
1:B:1380:LEU:HA	1:B:1381:PRO:HD3	1.88	0.41
1:A:327:ASP:OD1	1:A:363:LYS:CE	2.69	0.41
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.01	0.41
1:A:579:ASN:C	1:A:579:ASN:ND2	2.77	0.41
1:A:680:LYS:NZ	3:A:860:PLP:C4A	2.84	0.41
1:B:1633:ASP:OD2	1:B:1633:ASP:C	2.63	0.41
1:B:1557:ILE:O	1:B:1559:PRO:HD3	2.21	0.41
1:B:1558:ASN:OD1	1:B:1560:SER:HB3	2.21	0.41
1:B:1832:LEU:O	1:B:1833:LYS:CG	2.69	0.41
1:A:194:PRO:CB	1:B:1049:ARG:HE	2.34	0.41
1:A:277:ARG:HD3	5:B:2098:HOH:O	2.21	0.41
1:A:555:VAL:HG12	1:A:556:LYS:N	2.36	0.41
1:B:1033:ARG:HD2	5:B:2359:HOH:O	2.20	0.41
1:B:1386:ARG:NH2	1:B:1432:GLU:OE1	2.47	0.41
1:B:1752:PRO:C	1:B:1754:GLN:H	2.28	0.41
1:A:761:ILE:O	1:A:765:LEU:HB2	2.21	0.41
1:B:1330:PRO:CB	1:B:1370:LYS:HZ2	2.34	0.41
1:B:1645:LEU:HD13	1:B:1652:LEU:HD13	2.02	0.41
1:A:536:LYS:HD3	5:A:2212:HOH:O	2.20	0.40
1:A:810:LYS:HD2	1:A:811:PHE:CE1	2.56	0.40
1:B:1174:TRP:CD2	1:B:1621:LYS:HG3	2.55	0.40
1:B:1274:ASN:HD22	1:B:1277:ARG:HH11	1.65	0.40
1:A:415:VAL:CG2	1:A:425:LEU:HD11	2.51	0.40
1:B:1715:ILE:HG22	5:B:2405:HOH:O	2.20	0.40
1:A:194:PRO:HD2	1:B:1049:ARG:NH2	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLY:C	1:A:205:LYS:HG3	2.46	0.40
1:A:459:HIS:O	1:A:463:VAL:HG23	2.22	0.40
1:A:167:ASN:ND2	5:A:2466:HOH:O	2.45	0.40
1:A:715:ILE:HD11	5:A:2441:HOH:O	2.20	0.40
1:B:1274:ASN:HA	1:B:1277:ARG:HB2	2.03	0.40
1:B:1568:LYS:O	1:B:1607:GLY:HA3	2.21	0.40
1:A:241:MET:HG2	1:A:243:LEU:HD13	2.04	0.40
1:A:427:ARG:HH21	1:A:470:ASP:CG	2.29	0.40
1:B:1317:GLY:O	1:B:1318:SER:O	2.40	0.40
1:B:1426:ARG:H	1:B:1426:ARG:HG2	1.69	0.40
1:B:1426:ARG:HH11	1:B:1426:ARG:HG3	1.87	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	800/846 (95%)	748 (94%)	39 (5%)	13 (2%)	7 4
1	B	800/846 (95%)	749 (94%)	38 (5%)	13 (2%)	7 4
All	All	1600/1692 (95%)	1497 (94%)	77 (5%)	26 (2%)	7 4

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	PHE
1	A	318	SER
1	B	1317	GLY
1	B	1320	ARG
1	B	1322	ALA
1	B	1326	PHE
1	B	1836	LEU

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	322	ALA
1	A	324	THR
1	A	325	VAL
1	B	1318	SER
1	A	326	PHE
1	A	477	ASP
1	B	1315	LYS
1	B	1435	GLY
1	B	1477	ASP
1	B	1594	PRO
1	B	1832	LEU
1	A	594	PRO
1	A	834	ILE
1	A	435	GLY
1	A	476	PRO
1	B	1324	THR
1	B	1476	PRO
1	A	321	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	702/739 (95%)	665 (95%)	37 (5%)	20	19
1	B	702/739 (95%)	669 (95%)	33 (5%)	23	24
All	All	1404/1478 (95%)	1334 (95%)	70 (5%)	22	22

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	78	CYS
1	A	90	TYR
1	A	95	LEU

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	104	LEU
1	A	209	THR
1	A	213	THR
1	A	214	LYS
1	A	243	LEU
1	A	278	VAL
1	A	299	VAL
1	A	319	THR
1	A	324	THR
1	A	337	LEU
1	A	382	GLU
1	A	422	VAL
1	A	426	ARG
1	A	434	GLU
1	A	499	LEU
1	A	502	LEU
1	A	543	LEU
1	A	551	THR
1	A	568	LYS
1	A	576	GLN
1	A	577	LEU
1	A	622	LEU
1	A	645	LEU
1	A	652	LEU
1	A	683	LEU
1	A	730	GLU
1	A	759	LYS
1	A	765	LEU
1	A	810	LYS
1	A	815	ARG
1	A	828	GLU
1	A	833	LYS
1	B	1023	ASN
1	B	1040	VAL
1	B	1049	ARG
1	B	1078	CYS
1	B	1095	LEU
1	B	1120	GLU
1	B	1243	LEU
1	B	1278	VAL
1	B	1299	VAL

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Mol	Chain	Res	Type
1	B	1337	LEU
1	B	1422	VAL
1	B	1426	ARG
1	B	1434	GLU
1	B	1499	LEU
1	B	1502	LEU
1	B	1543	LEU
1	B	1551	THR
1	B	1568	LYS
1	B	1576	GLN
1	B	1577	LEU
1	B	1622	LEU
1	B	1645	LEU
1	B	1652	LEU
1	B	1683	LEU
1	B	1730	GLU
1	B	1759	LYS
1	B	1765	LEU
1	B	1772	LYS
1	B	1810	LYS
1	B	1815	ARG
1	B	1828	GLU
1	B	1831	ASP
1	B	1832	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	34	HIS
1	A	62	HIS
1	A	72	GLN
1	A	73	HIS
1	A	96	GLN
1	A	114	GLN
1	A	167	ASN
1	A	168	GLN
1	A	236	ASN
1	A	239	ASN
1	A	270	ASN
1	A	274	ASN
1	A	341	HIS

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Mol	Chain	Res	Type
1	A	450	HIS
1	A	481	ASN
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	614	HIS
1	A	763	ASN
1	A	768	HIS
1	A	804	ASN
1	A	822	GLN
1	B	1023	ASN
1	B	1032	ASN
1	B	1034	HIS
1	B	1062	HIS
1	B	1073	HIS
1	B	1105	GLN
1	B	1106	ASN
1	B	1114	GLN
1	B	1167	ASN
1	B	1168	GLN
1	B	1210	ASN
1	B	1236	ASN
1	B	1239	ASN
1	B	1270	ASN
1	B	1274	ASN
1	B	1450	HIS
1	B	1459	HIS
1	B	1481	ASN
1	B	1541	ASN
1	B	1547	GLN
1	B	1566	GLN
1	B	1576	GLN
1	B	1579	ASN
1	B	1614	HIS
1	B	1763	ASN
1	B	1768	HIS
1	B	1822	GLN

5.3.3 RNA ⓘ

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](#)

6 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	NBG	B	1861	-	15,15,15	1.67	3 (20%)	21,21,21	1.31	2 (9%)
4	288	A	862	-	27,27,27	2.35	4 (14%)	32,37,37	1.63	8 (25%)
4	288	B	1862	-	27,27,27	2.42	3 (11%)	32,37,37	1.51	7 (21%)
3	PLP	B	1860	-	15,15,16	2.49	4 (26%)	21,22,23	1.28	1 (4%)
3	PLP	A	860	-	15,15,16	2.57	6 (40%)	21,22,23	1.30	2 (9%)
2	NBG	A	861	-	15,15,15	1.43	3 (20%)	21,21,21	1.34	2 (9%)

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	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
4	288	A	862	-	1/1/4/5	4/18/27/27	0/3/3/3
4	288	B	1862	-	1/1/4/5	3/18/27/27	0/3/3/3
3	PLP	B	1860	-	-	0/6/6/8	0/1/1/1
3	PLP	A	860	-	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	288	O17-C15	-11.10	1.21	1.41
4	A	862	288	O17-C15	-10.50	1.22	1.41
3	B	1860	PLP	C4A-C4	-7.50	1.36	1.51
3	A	860	PLP	C4A-C4	-7.32	1.37	1.51
2	B	1861	NBG	C2-C1	4.15	1.57	1.53
3	B	1860	PLP	C3-C2	-3.60	1.37	1.41
2	A	861	NBG	C2-C1	3.53	1.56	1.53
3	A	860	PLP	C3-C2	-3.43	1.37	1.41
3	A	860	PLP	C2A-C2	3.30	1.55	1.50
2	B	1861	NBG	C1-N1	3.14	1.47	1.43
3	A	860	PLP	P-O2P	-2.48	1.45	1.54
4	B	1862	288	C19-N16	2.41	1.50	1.46
2	B	1861	NBG	C3-C2	2.37	1.58	1.52
4	A	862	288	C10-N12	2.29	1.37	1.33
4	A	862	288	C19-N16	2.25	1.50	1.46
3	A	860	PLP	C5A-C5	2.22	1.56	1.50
3	A	860	PLP	P-O3P	-2.21	1.46	1.54
2	A	861	NBG	C3-C2	2.12	1.57	1.52
3	B	1860	PLP	C5-C4	-2.10	1.38	1.40
3	B	1860	PLP	C2A-C2	2.08	1.53	1.50
4	B	1862	288	C1-C2	2.03	1.44	1.41
2	A	861	NBG	C1-N1	2.02	1.46	1.43
4	A	862	288	C9-C8	2.01	1.41	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	NBG	C5-O5-C1	4.58	118.83	112.47
2	B	1861	NBG	C5-O5-C1	4.49	118.71	112.47
4	A	862	288	C7-C10-N12	4.34	122.77	116.80
4	B	1862	288	C7-C10-N12	3.97	122.26	116.80
4	B	1862	288	O17-C15-C14	3.94	119.34	108.69
4	A	862	288	O17-C15-C14	3.91	119.26	108.69
3	A	860	PLP	O2P-P-O4P	-3.29	98.08	106.67
4	A	862	288	C14-N12-C10	-3.05	117.47	122.06
4	B	1862	288	C19-N16-C18	2.80	120.56	114.20
4	A	862	288	C19-N16-C18	2.78	120.53	114.20
3	A	860	PLP	O3P-P-O2P	2.56	117.42	107.80
4	A	862	288	O13-C10-C7	-2.49	117.88	121.09
4	A	862	288	C6-C2-C1	-2.39	119.97	122.13
4	B	1862	288	O13-C10-C7	-2.35	118.06	121.09
4	B	1862	288	C6-C2-C1	-2.34	120.01	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	288	O13-C10-N12	-2.22	119.35	123.35
2	A	861	NBG	C2-C1-N1	-2.18	108.44	111.25
4	A	862	288	C19-N16-C15	2.17	120.79	114.34
3	B	1860	PLP	O3P-P-O4P	-2.16	101.04	106.67
2	B	1861	NBG	C3-C2-C1	2.11	112.95	109.86
4	B	1862	288	O13-C10-N12	-2.03	119.68	123.35
4	B	1862	288	C19-N16-C15	2.02	120.36	114.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	862	288	C15
4	B	1862	288	C15

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	862	288	N12-C14-C15-O17
4	A	862	288	C14-C15-N16-C19
4	B	1862	288	N12-C14-C15-O17
4	B	1862	288	C14-C15-N16-C19
4	A	862	288	C14-C15-N16-C18
4	B	1862	288	C14-C15-N16-C18
4	A	862	288	C21-C18-N16-C15

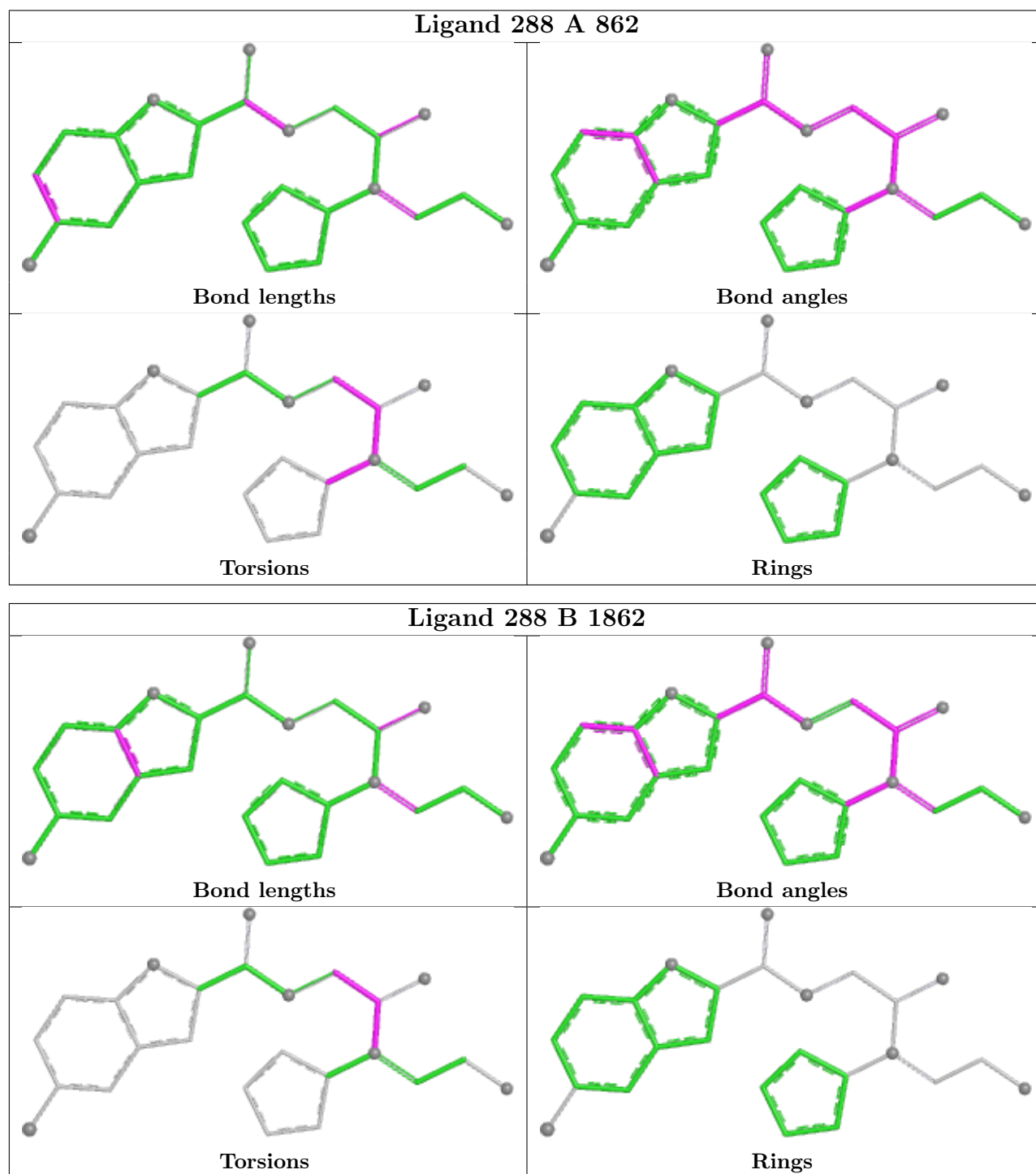
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1862	288	3	0
3	A	860	PLP	1	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.