



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:43 am GMT

PDB ID : 2IUK
Title : Crystal structure of Soybean Lipxygenase-D
Authors : Youn, B.; Sellhorn, G.E.; Mirchel, R.J.; Gaffney, B.J.; Grimes, H.D.; Kang, C.
Deposited on : 2006-06-05
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

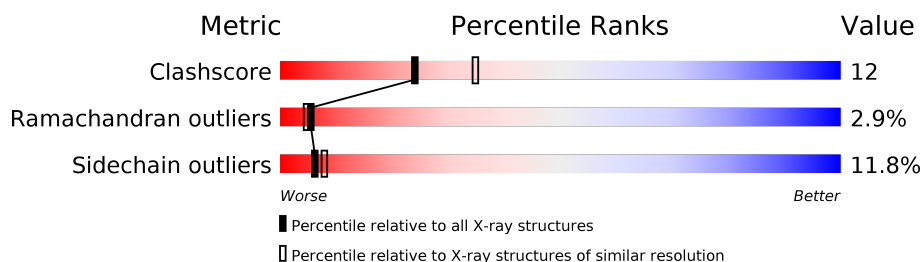
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	864	
1	B	864	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13534 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 SEED LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			
1	B	835	Total	C	N	O	S	0	0	0
			6649	4272	1115	1251	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	PHE	LEU	CONFLICT	UNP P24095
A	233	CYS	SER	CONFLICT	UNP P24095
A	240	LEU	ARG	CONFLICT	UNP P24095
A	364	VAL	TRP	CONFLICT	UNP P24095
A	604	HIS	ASP	CONFLICT	UNP P24095
A	695	LYS	MET	CONFLICT	UNP P24095
B	1192	PHE	LEU	CONFLICT	UNP P24095
B	1233	CYS	SER	CONFLICT	UNP P24095
B	1240	LEU	ARG	CONFLICT	UNP P24095
B	1364	VAL	TRP	CONFLICT	UNP P24095
B	1604	HIS	ASP	CONFLICT	UNP P24095
B	1695	LYS	MET	CONFLICT	UNP P24095

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

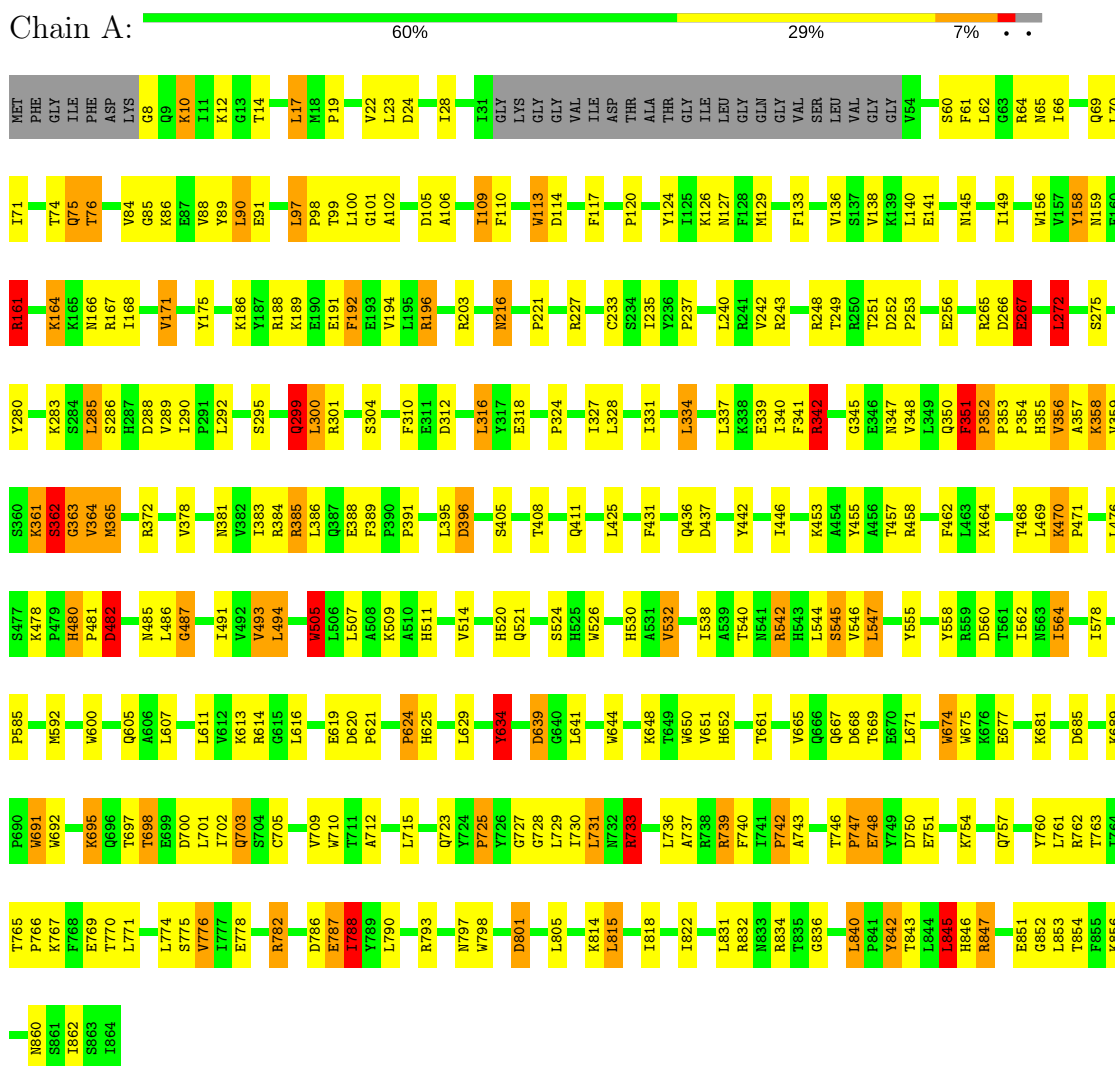
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	113	Total 113	O 113	0	0

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: SEED LIPOXYGENASE



• Molecule 1: SEED LIPOXYGENASE



D1773	A1678	L1486	G1586	L1486	M1379	Y1262	Y1163	Q1069	MET
V1776	V1679	G1487	K1587	G1487	P1380	V1263	K1164	L1070	PHE
I1777	E1680	P1488	S1589	P1488	N1381	R1264	R1265	I1071	GLY
E1778	G1682	V1493	L1494	V1493	V1382	R1265	Y1175	S1072	ILE
S1781	H1683	M1592	M1592	L1494	R1385	L1272	T1180	A1073	PHE
R1782	K1689	V1596	Y1597	P1496	A1496	K1273	P1181	T1074	ASP
L1790	P1690	Y1597	Y1597	G1499	S1393	S1274	A1182	Q1075	LYS
R1793	W1691	W1600	W1600	G1499	D1396	L1278	P1183	T1076	GLY
E1794	W1692	V1601	V1601	V1500	P1397	L1278	P1183	G1080	K1012
E1794	K1694	P1602	P1602	D1501	P1397	L1282	L1184	N1081	V1015
T1795	K1695	T1503	T1503	S1502	Y1400	K1283	L1185	G1082	V1016
P1796	T1607	I1504	I1504	T1503	Y1400	S1284	K1186	L1017	L1017
N1797	P1608	W1505	W1505	W1504	K1409	D1288	E1191	M1018	M1018
W1798	L1611	L1506	L1506	L1504	E1410	D1288	F1192	P1019	K1020
D1801	L1617	L1507	L1507	L1507	Q1411	S1315	L1195	D1024	D1024
K1802	A1617	A1508	A1508	A1508	I1414	E1318	G1201	I1028	I1028
K1803	A1617	K1509	K1509	K1509	I1414	E1318	K1202	T1029	T1029
K1809	D1620	V1512	V1512	V1512	V1421	I1321	G1201	S1030	S1030
R1810	P1621	S1517	S1517	S1517	V1421	K1322	K1202	I1031	I1031
L1815	P1624	Q1521	Q1521	Q1521	L1425	L1323	R1208	GLY	GLY
E1819	H1625	L1522	L1522	L1522	R1429	L1328	D1211	LYS	LYS
I1822	L1627	V1523	V1523	V1523	L1430	L1328	Y1212	GLY	GLY
L1831	V1630	S1524	S1524	S1524	F1431	I1331	Y1215	VAL	VAL
R1832	I1631	W1526	W1526	W1526	Q1436	S1332	N1216	ILE	ILE
N1833	E1632	L1527	L1527	L1527	I1440	P1333	D1222	ASP	ASP
T1835	D1633	W1528	W1528	W1528	I1440	L1334	R1227	THR	THR
G1836	Y1634	H1530	H1530	H1530	L1443	P1335	C1233	ALA	ALA
P1837	L1641	A1531	A1531	A1531	T1444	K1338	S1234	THR	THR
V1838	W1644	W1533	W1533	W1533	R1445	E1339	I1235	ILE	ILE
Q1839	I1647	T1540	T1540	T1540	I1446	I1340	I1235	LEU	LEU
Y1842	W1650	L1544	L1544	L1544	N1447	F1341	Y1236	GLY	GLY
T1843	V1651	D1560	D1560	D1560	S1448	R1342	F1237	GLN	GLN
L1844	Y1654	T1561	T1561	T1561	L1450	T1343	Y1238	VAL	VAL
L1845	V1655	I1562	I1562	I1562	R1458	E1346	R1241	SER	SER
R1847	L1657	N1563	N1563	N1563	G1467	N1347	V1242	LEU	LEU
S1848	L1657	I1564	I1564	I1564	T1468	V1348	F1128	VAL	VAL
S1849	V1665	N1565	N1565	N1565	K1470	L1349	M1129	GLY	GLY
E1850	D1668	L1567	L1567	L1567	P1471	H1355	F1134	V1054	V1054
L1853	T1669	Q1570	Q1570	Q1570	E1475	K1358	L1135	I1055	I1055
K1856	Q1672	A1575	A1575	A1575	L1476	V1359	V1138	D1056	D1056
I1862	W1673	D1576	D1576	D1576	S1477	D1252	K1139	T1059	T1059
S1863	W1674	G1577	G1577	G1577	S1477	S1255	L1140	S1060	S1060
I1864	W1675	I1578	I1578	I1578	H1480	E1256	E1141	F1061	F1061
	R1762	K1676	K1676	K1676	P1481	K1364	D1142	L1062	L1062
	T1763	E1677	E1677	E1677	D1482	V1257	W1156	G1063	G1063
					G1483	P1258	V1157	R1064	R1064
					D1484	G1259	Y1158	H1065	H1065
					A1371	E1260	N1159	T1066	T1066
					N1485	R1372	F1160	S1067	S1067
								M1068	M1068

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.76Å 115.10Å 120.22Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.1 (50.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13534	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: FE

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	0.84	3/6822 (0.0%)	1.66	136/9280 (1.5%)
1	B	0.83	1/6822 (0.0%)	1.58	92/9280 (1.0%)
All	All	0.84	4/13644 (0.0%)	1.62	228/18560 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	GLU	CB-CG	6.92	1.65	1.52
1	A	639	ASP	CA-CB	6.04	1.67	1.53
1	A	851	GLU	CG-CD	5.35	1.59	1.51
1	B	1798	TRP	CG-CD2	-5.23	1.34	1.43

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	SER	CA-C-N	-13.93	88.34	116.20
1	A	542	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	A	486	LEU	CA-C-N	-11.70	92.81	116.20
1	A	834	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	B	1793	ARG	NE-CZ-NH1	10.16	125.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	TRP	CD1-CG-CD2	9.75	114.10	106.30
1	B	1793	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	113	TRP	CE2-CD2-CG	-9.30	99.86	107.30
1	A	733	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	542	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	113	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	A	505	TRP	CE2-CD2-CG	-8.85	100.22	107.30
1	A	600	TRP	CD1-CG-CD2	8.82	113.35	106.30
1	A	692	TRP	CE2-CD2-CG	-8.77	100.29	107.30
1	A	644	TRP	CD1-CG-CD2	8.71	113.27	106.30
1	A	650	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	B	1600	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	342	ARG	CA-C-N	-8.60	98.29	117.20
1	B	1113	TRP	CE2-CD2-CG	-8.48	100.51	107.30
1	B	1710	TRP	CE2-CD2-CG	-8.47	100.52	107.30
1	A	692	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	B	1505	TRP	CE2-CD2-CG	-8.43	100.56	107.30
1	A	156	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	A	192	PHE	CB-CG-CD2	-8.41	114.92	120.80
1	B	1675	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	A	481	PRO	CA-C-N	-8.34	98.85	117.20
1	A	675	TRP	CD1-CG-CD2	8.32	112.96	106.30
1	A	505	TRP	CG-CD2-CE3	8.30	141.37	133.90
1	B	1644	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	B	1644	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	A	196	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	1650	TRP	CE2-CD2-CG	-8.22	100.72	107.30
1	B	1710	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	B	1113	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	1674	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	B	1526	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	B	1156	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	852	GLY	CA-C-N	-8.09	99.39	117.20
1	A	644	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	A	505	TRP	NE1-CE2-CZ2	-8.04	121.56	130.40
1	B	1526	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A	675	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	A	691	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	A	17	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	600	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	A	798	TRP	CE2-CD2-CG	-7.82	101.04	107.30
1	B	1156	TRP	CE2-CD2-CG	-7.81	101.05	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1650	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	A	526	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B	1674	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	A	299	GLN	CA-CB-CG	7.74	130.43	113.40
1	A	733	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	710	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	B	1600	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	A	674	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	A	710	TRP	CD1-CG-CD2	7.58	112.37	106.30
1	A	384	ARG	CA-CB-CG	7.56	130.04	113.40
1	B	1359	VAL	N-CA-C	-7.55	90.61	111.00
1	B	1834	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	526	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	B	1675	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	481	PRO	N-CA-C	7.36	131.24	112.10
1	A	692	TRP	CG-CD2-CE3	7.35	140.51	133.90
1	A	691	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	A	674	TRP	CG-CD2-CE3	7.30	140.47	133.90
1	B	1850	GLU	CA-CB-CG	7.30	129.47	113.40
1	B	1691	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	B	1117	PHE	N-CA-C	-7.26	91.39	111.00
1	A	798	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	267	GLU	CA-CB-CG	-7.21	97.54	113.40
1	B	1365	MET	N-CA-C	7.21	130.45	111.00
1	A	505	TRP	CB-CG-CD1	-7.17	117.68	127.00
1	A	614	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	357	ALA	C-N-CA	7.10	139.46	121.70
1	B	1505	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	B	1192	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	B	1505	TRP	CB-CG-CD1	-7.01	117.89	127.00
1	B	1449	LEU	N-CA-CB	-7.00	96.41	110.40
1	A	76	THR	N-CA-CB	-6.99	97.03	110.30
1	A	639	ASP	CA-CB-CG	6.97	128.73	113.40
1	B	1175	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	A	156	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	762	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	442	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	B	1842	TYR	CB-CG-CD1	-6.82	116.91	121.00
1	B	1030	SER	CA-C-N	-6.82	102.21	117.20
1	B	1243	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	691	TRP	CG-CD2-CE3	6.77	139.99	133.90
1	A	256	GLU	CA-CB-CG	6.76	128.28	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1650	TRP	CB-CG-CD1	-6.76	118.22	127.00
1	A	486	LEU	O-C-N	6.75	134.68	123.20
1	B	1526	TRP	CG-CD2-CE3	6.74	139.97	133.90
1	B	1692	TRP	CE2-CD2-CG	-6.74	101.91	107.30
1	A	650	TRP	CB-CG-CD1	-6.72	118.27	127.00
1	B	1208	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	1634	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	B	1650	TRP	CG-CD2-CE3	6.59	139.84	133.90
1	A	486	LEU	C-N-CA	6.57	136.10	122.30
1	A	272	LEU	CA-CB-CG	6.55	130.36	115.30
1	B	1602	PHE	CA-CB-CG	6.52	129.54	113.90
1	B	1782	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	1505	TRP	CG-CD2-CE3	6.49	139.75	133.90
1	A	555	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	B	1602	PHE	CB-CG-CD1	6.47	125.33	120.80
1	B	1481	PRO	C-N-CA	6.46	137.85	121.70
1	A	342	ARG	O-C-N	6.41	132.96	122.70
1	B	1692	TRP	CA-CB-CG	6.39	125.84	113.70
1	A	362	SER	O-C-N	6.39	134.06	123.20
1	A	692	TRP	CB-CG-CD1	-6.32	118.79	127.00
1	B	1449	LEU	CB-CA-C	6.27	122.11	110.20
1	A	482	ASP	CA-C-N	6.25	128.69	116.20
1	A	97	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	851	GLU	CB-CG-CD	6.20	130.94	114.20
1	B	1248	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	1691	TRP	CD1-CG-CD2	6.18	111.24	106.30
1	A	240	LEU	CB-CA-C	6.17	121.92	110.20
1	A	505	TRP	NE1-CE2-CD2	6.15	113.45	107.30
1	A	691	TRP	CB-CG-CD1	-6.12	119.04	127.00
1	B	1723	GLN	N-CA-CB	-6.09	99.63	110.60
1	B	1592	MET	CG-SD-CE	-6.08	90.47	100.20
1	A	505	TRP	CA-CB-CG	-6.07	102.17	113.70
1	B	1596	VAL	CG1-CB-CG2	-6.07	101.19	110.90
1	A	300	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	363	GLY	N-CA-C	-6.05	97.98	113.10
1	A	852	GLY	O-C-N	6.05	132.37	122.70
1	B	1669	THR	CA-CB-CG2	6.02	120.83	112.40
1	B	1113	TRP	CB-CG-CD1	-6.00	119.21	127.00
1	B	1798	TRP	CE2-CD2-CG	-5.99	102.51	107.30
1	A	834	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	487	GLY	N-CA-C	-5.96	98.21	113.10
1	A	644	TRP	CG-CD2-CE3	5.95	139.25	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1448	SER	CA-C-N	-5.91	104.20	117.20
1	A	698	THR	CA-CB-CG2	5.91	120.67	112.40
1	A	731	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	272	LEU	N-CA-C	-5.86	95.18	111.00
1	B	1191	GLU	CA-C-N	-5.84	104.34	117.20
1	B	1429	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	A	167	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	650	TRP	CG-CD2-CE3	5.78	139.10	133.90
1	B	1798	TRP	CD1-CG-CD2	5.74	110.89	106.30
1	B	1243	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	1062	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	1853	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	74	THR	CA-CB-CG2	5.69	120.37	112.40
1	A	674	TRP	CD1-CG-CD2	5.69	110.85	106.30
1	A	851	GLU	CA-CB-CG	5.68	125.90	113.40
1	A	171	VAL	CB-CA-C	-5.67	100.62	111.40
1	B	1113	TRP	CG-CD2-CE3	5.67	139.00	133.90
1	A	365	MET	CA-CB-CG	5.65	122.91	113.30
1	B	1163	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	762	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	600	TRP	CG-CD1-NE1	-5.64	104.45	110.10
1	A	639	ASP	CA-C-N	-5.64	104.93	116.20
1	A	188	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	316	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	1644	TRP	CG-CD2-CE3	5.60	138.94	133.90
1	B	1215	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	B	1692	TRP	CD1-CG-CD2	5.59	110.78	106.30
1	A	486	LEU	CA-C-O	5.59	131.84	120.10
1	A	113	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	A	546	VAL	CA-CB-CG2	-5.58	102.53	110.90
1	B	1142	ASP	CA-CB-CG	5.58	125.67	113.40
1	A	600	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	A	243	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	592	MET	CG-SD-CE	-5.55	91.31	100.20
1	A	650	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	A	845	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	227	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	1526	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	A	365	MET	N-CA-C	5.49	125.81	111.00
1	A	532	VAL	CA-CB-CG2	-5.46	102.70	110.90
1	A	832	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	1532	VAL	N-CA-CB	-5.45	99.51	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	788	ILE	CG1-CB-CG2	-5.45	99.42	111.40
1	A	787	GLU	N-CA-C	5.44	125.68	111.00
1	A	675	TRP	CG-CD2-CE3	5.43	138.79	133.90
1	A	362	SER	CA-C-O	5.42	131.47	120.10
1	B	1810	ARG	CA-CB-CG	5.41	125.31	113.40
1	A	592	MET	CA-CB-CG	-5.41	104.11	113.30
1	A	845	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	B	1575	ALA	CA-C-N	-5.39	105.34	117.20
1	B	1674	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B	1227	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	85	GLY	CA-C-N	-5.37	105.38	117.20
1	A	358	LYS	N-CA-C	-5.36	96.54	111.00
1	A	266	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	733	ARG	CG-CD-NE	5.33	123.00	111.80
1	B	1342	ARG	CA-C-N	-5.33	105.47	117.20
1	B	1339	GLU	CA-CB-CG	5.32	125.11	113.40
1	B	1324	PRO	CA-C-N	-5.29	105.55	117.20
1	B	1600	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	1505	TRP	NE1-CE2-CZ2	-5.28	124.59	130.40
1	B	1533	MET	CA-CB-CG	5.26	122.24	113.30
1	B	1164	LYS	CA-CB-CG	5.25	124.95	113.40
1	B	1030	SER	O-C-N	5.21	131.04	122.70
1	B	1715	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	481	PRO	C-N-CA	5.21	134.71	121.70
1	A	493	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	A	854	THR	N-CA-C	5.20	125.03	111.00
1	A	651	VAL	CG1-CB-CG2	-5.20	102.59	110.90
1	B	1669	THR	CA-CB-OG1	-5.19	98.11	109.00
1	A	156	TRP	CG-CD1-NE1	-5.17	104.92	110.10
1	B	1483	GLY	CA-C-N	-5.17	105.82	117.20
1	A	634	TYR	N-CA-C	-5.17	97.04	111.00
1	B	1512	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	B	1654	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	A	600	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	B	1567	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	782	ARG	CG-CD-NE	5.14	122.60	111.80
1	A	815	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	845	LEU	CB-CA-C	-5.12	100.47	110.20
1	A	300	LEU	N-CA-C	-5.12	97.19	111.00
1	A	760	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	B	1802	LYS	CA-CB-CG	5.11	124.64	113.40
1	A	339	GLU	CA-CB-CG	5.11	124.63	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	437	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	74	THR	CA-CB-OG1	-5.09	98.31	109.00
1	A	698	THR	CA-CB-OG1	-5.09	98.32	109.00
1	A	505	TRP	CD1-CG-CD2	5.08	110.37	106.30
1	A	385	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	114	ASP	CA-CB-CG	5.06	124.54	113.40
1	A	542	ARG	CA-CB-CG	5.05	124.51	113.40
1	A	75	GLN	CA-C-N	-5.04	106.10	117.20
1	B	1483	GLY	O-C-N	5.04	130.76	122.70
1	A	345	GLY	C-N-CA	5.02	134.26	121.70
1	A	240	LEU	O-C-N	-5.02	114.67	122.70
1	B	1496	ALA	CA-C-N	-5.01	106.19	117.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PHE	Peptide
1	A	362	SER	Mainchain
1	A	480	HIS	Peptide
1	A	487	GLY	Peptide
1	A	842	TYR	Sidechain
1	A	97	LEU	Peptide
1	B	1097	LEU	Peptide
1	B	1332	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6649	0	6597	153	0
1	B	6649	0	6597	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	121	0	0	5	0
3	B	113	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13534	0	13194	331	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 12.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HE	1:A:342:ARG:HA	1.31	0.94
1:A:847:ARG:H	1:A:847:ARG:NE	1.71	0.88
1:B:1020:LYS:H	1:B:1020:LYS:HD3	1.41	0.83
1:B:1371:ALA:HB2	1:B:1471:PRO:HD3	1.59	0.83
1:A:249:THR:HG22	1:A:252:ASP:H	1.43	0.81
1:B:1480:HIS:HD2	1:B:1486:LEU:HD23	1.45	0.80
1:B:1815:LEU:HB3	1:B:1847:ARG:HD2	1.64	0.78
1:A:847:ARG:H	1:A:847:ARG:HE	1.30	0.77
1:A:457:THR:HG22	1:A:476:LEU:HD23	1.68	0.75
1:B:1249:THR:HG22	1:B:1252:ASP:H	1.53	0.74
1:A:736:LEU:HD11	1:A:769:GLU:HG2	1.67	0.74
1:A:822:ILE:HG21	1:A:845:LEU:HD13	1.71	0.72
1:B:1847:ARG:H	1:B:1847:ARG:NE	1.87	0.72
1:A:743:ALA:O	1:A:746:THR:HB	1.90	0.70
1:A:822:ILE:HD12	1:A:845:LEU:HD22	1.71	0.70
1:B:1832:ARG:HA	1:B:1832:ARG:HE	1.56	0.69
1:A:846:HIS:HA	1:A:847:ARG:HH11	1.58	0.69
1:A:845:LEU:H	1:A:845:LEU:HD12	1.59	0.67
1:B:1411:GLN:HB3	1:B:1494:LEU:HD21	1.78	0.65
1:A:464:LYS:HD2	1:A:470:LYS:HB2	1.77	0.64
1:A:478:LYS:HD3	1:A:740:PHE:CE1	2.32	0.64
1:B:1607:LEU:HD13	1:B:1641:LEU:HD13	1.80	0.64
1:A:359:VAL:HG12	1:A:362:SER:H	1.62	0.64
1:B:1064:ARG:HA	1:B:1089:TYR:CD1	2.33	0.64
1:B:1711:THR:HA	1:B:1715:LEU:HB2	1.80	0.63
1:B:1059:THR:HB	1:B:1062:LEU:HD21	1.81	0.63
1:A:361:LYS:HD2	1:A:361:LYS:H	1.63	0.63
1:A:267:GLU:HG2	1:A:562:ILE:HB	1.80	0.63
1:B:1471:PRO:HB2	1:B:1505:TRP:HH2	1.63	0.63
1:A:334:LEU:HD23	1:A:337:LEU:HD13	1.81	0.63
1:A:507:LEU:HD13	1:A:739:ARG:HH22	1.63	0.63
1:A:331:ILE:HA	1:A:334:LEU:HD22	1.81	0.62
1:B:1703:GLN:O	1:B:1707:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:GLU:O	1:A:782:ARG:HD3	2.00	0.61
1:A:69:GLN:HE21	1:A:124:TYR:HD2	1.48	0.61
1:A:355:HIS:HB3	1:A:840:LEU:HD21	1.81	0.61
1:B:1127:ASN:O	1:B:1159:ASN:HA	1.99	0.61
1:B:1103:ARG:H	1:B:1103:ARG:HD3	1.66	0.60
1:B:1525:HIS:O	1:B:1529:THR:HB	2.01	0.60
1:A:408:THR:H	1:A:411:GLN:HE21	1.50	0.60
1:B:1328:LEU:HD23	1:B:1331:ILE:HD12	1.82	0.60
1:B:1845:LEU:HD23	3:B:2113:HOH:O	2.02	0.60
1:B:1485:ASN:C	1:B:1487:GLY:H	2.04	0.60
1:A:471:PRO:HB2	1:A:505:TRP:HH2	1.66	0.60
1:A:295:SER:O	1:A:299:GLN:HB3	2.01	0.59
1:A:695:LYS:HD3	3:A:2038:HOH:O	2.01	0.59
1:A:248:ARG:HD2	1:A:253:PRO:O	2.01	0.59
1:A:285:LEU:HD12	1:A:776:VAL:HG13	1.85	0.59
1:A:471:PRO:HB2	1:A:505:TRP:CH2	2.38	0.58
1:B:1443:LEU:HA	1:B:1446:ILE:HG12	1.84	0.58
1:A:386:LEU:HD21	1:A:391:PRO:HG3	1.84	0.58
1:B:1713:SER:HB2	1:B:1790:LEU:HG	1.85	0.58
1:A:695:LYS:HE2	1:A:701:LEU:HA	1.85	0.58
1:B:1608:PRO:HB3	1:B:1627:LEU:HD11	1.86	0.58
1:B:1097:LEU:HD22	1:B:1105:ASP:HA	1.86	0.58
1:B:1101:GLY:O	1:B:1103:ARG:HD3	2.04	0.57
1:B:1095:PRO:C	1:B:1097:LEU:H	2.06	0.57
1:B:1611:LEU:HB3	1:B:1617:ALA:HB2	1.86	0.57
1:B:1015:VAL:HG22	1:B:1138:VAL:HG22	1.86	0.57
1:B:1782:ARG:CZ	1:B:1853:LEU:HA	2.34	0.57
1:B:1202:LYS:HG2	3:B:2035:HOH:O	2.04	0.57
1:A:530:HIS:CE1	1:A:564:ILE:HD13	2.39	0.57
1:A:668:ASP:HB3	3:A:2100:HOH:O	2.05	0.57
1:B:1249:THR:HB	1:B:1252:ASP:O	2.04	0.57
1:B:1015:VAL:HG12	1:B:1017:LEU:HD23	1.85	0.57
1:A:310:PHE:H	1:A:757:GLN:NE2	2.02	0.56
1:B:1020:LYS:N	1:B:1020:LYS:HD3	2.14	0.56
1:B:1447:ASN:C	1:B:1449:LEU:H	2.07	0.56
1:A:71:ILE:HG12	1:A:84:VAL:HG12	1.86	0.56
1:A:677:GLU:HG3	1:A:681:LYS:HE3	1.87	0.56
1:B:1233:CYS:HB2	1:B:1236:TYR:HB2	1.88	0.56
1:A:616:LEU:HG	1:A:634:TYR:HE1	1.70	0.56
1:A:538:ILE:O	1:A:542:ARG:HG3	2.06	0.55
1:B:1843:THR:HB	1:B:1856:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ASP:O	1:A:754:LYS:HG2	2.06	0.55
1:B:1654:TYR:HB3	3:B:2096:HOH:O	2.06	0.55
1:A:446:ILE:HG12	1:A:585:PRO:HA	1.88	0.55
1:A:733:ARG:HB3	1:A:733:ARG:HH11	1.71	0.55
1:B:1607:LEU:HG	1:B:1710:TRP:CZ2	2.40	0.55
1:B:1527:LEU:O	1:B:1532:VAL:HB	2.07	0.55
1:B:1540:THR:HG23	1:B:1544:LEU:HD12	1.89	0.55
1:B:1657:LEU:HD22	1:B:1803:LYS:HD2	1.88	0.55
1:A:272:LEU:HD22	1:A:272:LEU:H	1.71	0.54
1:B:1750:ASP:O	1:B:1754:LYS:HD3	2.07	0.54
1:A:770:THR:O	1:A:774:LEU:HG	2.07	0.54
1:B:1530:HIS:CE1	1:B:1564:ILE:HD13	2.42	0.54
1:B:1602:PHE:HB3	3:B:2081:HOH:O	2.07	0.54
1:B:1445:ARG:NE	1:B:1445:ARG:HA	2.22	0.54
1:B:1529:THR:CG2	1:B:1716:HIS:HD2	2.19	0.54
1:A:493:VAL:HG12	1:A:505:TRP:HD1	1.71	0.54
1:B:1443:LEU:HD23	1:B:1446:ILE:HD11	1.90	0.54
1:A:846:HIS:HA	1:A:847:ARG:NH1	2.21	0.53
1:A:822:ILE:HG23	1:A:845:LEU:HD22	1.90	0.53
1:A:12:LYS:HB3	1:A:141:GLU:HB2	1.89	0.53
1:B:1493:VAL:HG21	1:B:1508:ALA:HB2	1.91	0.53
1:A:767:LYS:O	1:A:771:LEU:HG	2.07	0.53
1:A:216:ASN:H	1:A:216:ASN:HD22	1.56	0.53
1:A:285:LEU:HD21	1:A:775:SER:HB3	1.90	0.53
1:B:1069:GLN:HG2	1:B:1124:TYR:HB2	1.91	0.53
1:A:342:ARG:NE	1:A:342:ARG:HA	2.04	0.53
1:B:1778:GLU:O	1:B:1782:ARG:HG2	2.09	0.52
1:B:1247:GLU:HG3	3:B:2040:HOH:O	2.09	0.52
1:A:520:HIS:HA	1:A:524:SER:HB2	1.91	0.52
1:A:544:LEU:HD13	1:A:674:TRP:HB2	1.91	0.52
1:B:1181:PRO:HB2	1:B:1184:LEU:HB2	1.92	0.52
1:B:1782:ARG:NH1	1:B:1853:LEU:HB3	2.24	0.52
1:A:100:LEU:HD21	1:A:106:ALA:HB2	1.91	0.52
1:B:1505:TRP:O	1:B:1509:LYS:HG3	2.10	0.52
1:B:1846:HIS:HA	1:B:1847:ARG:NH1	2.25	0.52
1:A:249:THR:HB	1:A:252:ASP:O	2.08	0.51
1:A:665:VAL:HG11	1:A:697:THR:O	2.09	0.51
1:A:88:VAL:HG11	1:A:110:PHE:O	2.10	0.51
1:B:1560:ASP:O	1:B:1564:ILE:HG13	2.11	0.51
1:A:639:ASP:HB2	1:A:845:LEU:HG	1.92	0.51
1:B:1201:GLY:O	1:B:1243:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1284:SER:O	1:B:1288:ASP:HB2	2.11	0.50
1:B:1675:TRP:CZ2	1:B:1693:PRO:HG2	2.46	0.50
1:B:1076:THR:HG22	1:B:1183:PRO:HG3	1.93	0.50
1:B:1530:HIS:HD1	1:B:1565:ASN:ND2	2.10	0.50
1:A:60:SER:C	1:A:62:LEU:H	2.15	0.50
1:B:1127:ASN:HD21	1:B:1129:MET:HB2	1.77	0.50
1:A:395:LEU:O	1:A:396:ASP:HB2	2.12	0.50
1:B:1815:LEU:O	1:B:1819:GLU:HG3	2.12	0.50
1:A:385:ARG:HG3	1:A:431:PHE:CE2	2.47	0.49
1:B:1759:ALA:O	1:B:1763:THR:HG23	2.12	0.49
1:A:14:THR:O	1:A:138:VAL:HA	2.12	0.49
1:A:196:ARG:HG2	1:A:542:ARG:HB3	1.93	0.49
1:A:540:THR:HG21	1:A:558:TYR:HE2	1.77	0.49
1:B:1449:LEU:HB3	1:B:1450:PRO:HA	1.93	0.49
1:B:1822:ILE:HD12	1:B:1847:ARG:HH12	1.77	0.49
1:A:629:LEU:HD22	3:A:2096:HOH:O	2.13	0.49
1:B:1342:ARG:HA	1:B:1342:ARG:NE	2.27	0.49
1:B:1689:LYS:O	1:B:1692:TRP:HD1	1.96	0.49
1:A:164:LYS:HD3	1:A:164:LYS:H	1.77	0.49
1:A:801:ASP:O	1:A:805:LEU:HG	2.13	0.49
1:A:126:LYS:HE2	1:A:166:ASN:HD21	1.77	0.49
1:B:1093:HIS:NE2	1:B:1097:LEU:HD21	2.28	0.49
1:A:66:ILE:HD12	1:A:133:PHE:CE2	2.48	0.48
1:A:712:ALA:HA	1:A:862:ILE:HG13	1.95	0.48
1:A:237:PRO:HA	1:A:685:ASP:OD2	2.13	0.48
1:B:1529:THR:HG21	1:B:1716:HIS:HD2	1.78	0.48
1:B:1020:LYS:CD	1:B:1020:LYS:H	2.14	0.48
1:B:1436:GLN:O	1:B:1440:ILE:HB	2.14	0.48
1:B:1315:SER:HA	1:B:1318:GLU:HB2	1.94	0.48
1:A:354:PRO:HB3	1:A:728:GLY:HA3	1.96	0.48
1:A:727:GLY:HA2	1:A:733:ARG:HB2	1.96	0.48
1:B:1698:THR:O	1:B:1702:ILE:HG13	2.14	0.48
1:B:1059:THR:O	1:B:1061:PHE:N	2.46	0.48
1:B:1216:ASN:HB2	1:B:1255:SER:HA	1.94	0.48
1:B:1370:PHE:HD2	1:B:1471:PRO:HG3	1.77	0.48
1:B:1458:ARG:HD2	1:B:1475:GLU:OE2	2.13	0.48
1:A:788:ILE:HG22	1:A:860:ASN:ND2	2.29	0.48
1:B:1081:ASN:OD1	1:B:1186:LYS:HD3	2.14	0.48
1:B:1530:HIS:HD1	1:B:1565:ASN:HD21	1.60	0.48
1:B:1202:LYS:HD3	1:B:1246:ARG:HA	1.96	0.48
1:B:1655:VAL:HG21	1:B:1702:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:HD12	3:A:2083:HOH:O	2.13	0.47
1:B:1355:HIS:HB2	1:B:1725:PRO:HA	1.95	0.47
1:B:1523:VAL:HG11	1:B:1596:VAL:HG11	1.95	0.47
1:A:372:ARG:HD2	1:A:836:GLY:HA3	1.95	0.47
1:A:192:PHE:HZ	1:A:545:SER:N	2.11	0.47
1:A:521:GLN:HE22	1:A:723:GLN:NE2	2.11	0.47
1:A:90:LEU:HA	1:A:109:ILE:HG23	1.96	0.47
1:B:1062:LEU:HD22	1:B:1062:LEU:H	1.80	0.47
1:B:1409:LYS:HA	1:B:1421:VAL:HG21	1.96	0.47
1:B:1723:GLN:HB3	1:B:1781:SER:OG	2.14	0.47
1:B:1561:THR:HG23	1:B:1862:ILE:HB	1.95	0.47
1:B:1322:LYS:HD3	1:B:1322:LYS:H	1.80	0.47
1:B:1443:LEU:O	1:B:1447:ASN:HB2	2.14	0.47
1:A:560:ASP:O	1:A:564:ILE:HG13	2.15	0.47
1:A:514:VAL:HG11	1:A:737:ALA:HB2	1.96	0.47
1:B:1521:GLN:HE22	1:B:1723:GLN:NE2	2.13	0.47
1:B:1602:PHE:CZ	1:B:1679:VAL:HG13	2.50	0.47
1:B:1602:PHE:HZ	1:B:1679:VAL:HG13	1.80	0.47
1:A:175:TYR:HD2	1:A:547:LEU:HG	1.80	0.46
1:B:1158:TYR:H	1:B:1163:TYR:HE1	1.61	0.46
1:A:124:TYR:HE1	1:A:168:ILE:HG12	1.80	0.46
1:A:822:ILE:HD12	1:A:845:LEU:CD2	2.44	0.46
1:B:1707:ILE:O	1:B:1711:THR:HG23	2.15	0.46
1:B:1282:ILE:HG21	1:B:1567:LEU:HD11	1.98	0.46
1:B:1493:VAL:HG23	1:B:1505:TRP:CD1	2.51	0.46
1:B:1607:LEU:HD22	1:B:1611:LEU:HD22	1.96	0.46
1:B:1675:TRP:HZ2	1:B:1693:PRO:HG2	1.79	0.46
1:A:75:GLN:HB2	1:A:117:PHE:O	2.16	0.46
1:A:842:TYR:O	1:A:845:LEU:HD11	2.16	0.46
1:B:1192:PHE:HA	1:B:1192:PHE:HD1	1.66	0.46
1:B:1597:TYR:OH	1:B:1683:HIS:HD2	1.98	0.46
1:B:1372:ARG:HD2	1:B:1836:GLY:HA3	1.98	0.46
1:B:1797:ASN:H	1:B:1797:ASN:ND2	2.13	0.46
1:A:65:ASN:ND2	1:A:129:MET:HG2	2.31	0.46
1:B:1529:THR:HG22	1:B:1530:HIS:N	2.30	0.46
1:A:671:LEU:HB3	3:A:2100:HOH:O	2.15	0.46
1:A:705:CYS:O	1:A:709:VAL:HG23	2.15	0.46
1:A:19:PRO:HG3	1:A:61:PHE:CZ	2.51	0.46
1:B:1261:VAL:HG23	1:B:1570:GLN:HE21	1.81	0.46
1:A:289:VAL:HG21	1:A:337:LEU:HD22	1.97	0.45
1:A:842:TYR:CE2	1:A:845:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:VAL:HG11	1:B:1563:ASN:HA	1.98	0.45
1:B:1028:ILE:HG22	1:B:1274:SER:HB3	1.99	0.45
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.70	0.45
1:B:1385:ARG:HA	1:B:1431:PHE:CD2	2.52	0.45
1:A:757:GLN:O	1:A:761:LEU:HD12	2.16	0.45
1:B:1071:ILE:HB	1:B:1122:ALA:HB3	1.97	0.45
1:A:233:CYS:SG	1:A:235:ILE:HB	2.57	0.45
1:B:1449:LEU:HB3	1:B:1450:PRO:CA	2.47	0.45
1:A:192:PHE:CZ	1:A:545:SER:N	2.85	0.45
1:B:1070:LEU:HD13	1:B:1120:PRO:HB3	1.98	0.45
1:B:1211:ASP:O	1:B:1242:VAL:HA	2.16	0.45
1:B:1477:SER:HB3	1:B:1488:PRO:HB2	1.99	0.45
1:A:191:GLU:O	1:A:194:VAL:HB	2.17	0.45
1:A:351:PHE:HB3	1:A:352:PRO:HA	1.99	0.45
1:A:359:VAL:HG12	1:A:362:SER:N	2.31	0.45
1:A:285:LEU:HD13	1:A:290:ILE:HD11	1.99	0.44
1:B:1061:PHE:HB3	1:B:1066:ILE:HD12	2.00	0.44
1:A:476:LEU:HD12	1:A:491:ILE:HD11	1.98	0.44
1:A:505:TRP:CE3	1:A:509:LYS:HD2	2.52	0.44
1:A:620:ASP:HA	1:A:621:PRO:HD3	1.80	0.44
1:A:355:HIS:ND1	1:A:725:PRO:HG3	2.33	0.44
1:A:765:THR:HA	1:A:766:PRO:HD2	1.80	0.44
1:A:124:TYR:CE1	1:A:168:ILE:HG12	2.52	0.44
1:B:1665:VAL:HG12	1:B:1695:LYS:O	2.17	0.44
1:B:1334:LEU:HA	1:B:1335:PRO:HD3	1.80	0.44
1:B:1607:LEU:HD22	1:B:1611:LEU:CD2	2.47	0.44
1:B:1668:ASP:O	1:B:1672:GLN:HB2	2.17	0.44
1:B:1819:GLU:HG2	1:B:1847:ARG:HE	1.83	0.44
1:B:1012:LYS:O	1:B:1140:LEU:HA	2.17	0.44
1:B:1797:ASN:H	1:B:1797:ASN:HD22	1.66	0.44
1:B:1094:LEU:CD1	1:B:1108:SER:HB2	2.48	0.44
1:B:1321:ILE:HG23	1:B:1349:LEU:HB3	2.00	0.44
1:A:19:PRO:O	1:A:22:VAL:HG22	2.18	0.43
1:A:24:ASP:O	1:A:28:ILE:HG13	2.18	0.43
1:A:364:VAL:HG22	1:A:365:MET:HG2	2.00	0.43
1:B:1358:LYS:HA	1:B:1358:LYS:HD3	1.68	0.43
1:B:1695:LYS:HE3	1:B:1701:LEU:HA	2.00	0.43
1:B:1712:ALA:HA	1:B:1862:ILE:HD11	2.00	0.43
1:A:159:ASN:OD1	1:A:161:ARG:HB2	2.18	0.43
1:A:470:LYS:HZ2	1:A:471:PRO:HD2	1.82	0.43
1:A:843:THR:O	1:A:856:LYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HA	1:A:89:TYR:CD2	2.54	0.43
1:B:1082:GLY:HA2	1:B:1183:PRO:HB3	2.00	0.43
1:B:1819:GLU:CG	1:B:1847:ARG:HE	2.31	0.43
1:B:1505:TRP:CE3	1:B:1509:LYS:HE2	2.54	0.43
1:A:248:ARG:HB3	1:A:253:PRO:HA	2.01	0.43
1:A:625:HIS:CD2	1:A:641:LEU:HD13	2.53	0.43
1:A:363:GLY:O	1:A:365:MET:N	2.52	0.43
1:A:648:LYS:HZ3	1:A:703:GLN:HG2	1.83	0.43
1:A:689:LYS:HD2	1:A:691:TRP:HE1	1.83	0.43
1:B:1641:LEU:HA	1:B:1641:LEU:HD12	1.92	0.43
1:A:411:GLN:HB3	1:A:494:LEU:HD11	2.01	0.43
1:A:511:HIS:CE1	1:A:737:ALA:HB1	2.54	0.43
1:B:1056:ASP:HB3	1:B:1059:THR:HG23	1.99	0.43
1:B:1467:GLY:O	1:B:1833:ASN:ND2	2.52	0.43
1:A:158:TYR:HE1	1:A:265:ARG:HG2	1.84	0.43
1:A:221:PRO:HG2	1:A:249:THR:HG21	2.01	0.43
1:A:639:ASP:HA	1:A:845:LEU:HD23	2.00	0.43
1:B:1822:ILE:HD12	1:B:1847:ARG:NH1	2.34	0.43
1:A:129:MET:HB2	1:A:129:MET:HE3	1.76	0.42
1:A:455:TYR:CD1	1:A:476:LEU:HB3	2.53	0.42
1:A:462:PHE:O	1:A:469:LEU:HA	2.19	0.42
1:B:1119:ILE:HA	1:B:1120:PRO:HD2	1.77	0.42
1:B:1396:ASP:HA	1:B:1397:PRO:HD3	1.86	0.42
1:B:1521:GLN:HE22	1:B:1723:GLN:HE22	1.65	0.42
1:A:299:GLN:CG	1:A:300:LEU:H	2.32	0.42
1:B:1018:MET:HB2	1:B:1134:PHE:HB3	2.02	0.42
1:B:1692:TRP:HA	1:B:1693:PRO:HD2	1.86	0.42
1:B:1061:PHE:HD2	1:B:1066:ILE:HD11	1.85	0.42
1:B:1679:VAL:HG11	1:B:1692:TRP:CE3	2.55	0.42
1:A:746:THR:HG22	1:A:748:GLU:HG2	2.00	0.42
1:A:739:ARG:HG3	1:A:763:THR:HA	2.01	0.42
1:B:1470:LYS:HE3	1:B:1470:LYS:HB2	1.87	0.42
1:B:1362:SER:OG	1:B:1837:PRO:HB2	2.20	0.42
1:A:280:TYR:HA	1:A:283:LYS:NZ	2.35	0.42
1:A:405:SER:HA	1:A:458:ARG:NH2	2.35	0.42
1:A:8:GLY:C	1:A:10:LYS:H	2.23	0.42
1:B:1073:ALA:HB2	1:B:1121:GLY:HA3	2.02	0.42
1:B:1742:PRO:HG2	1:B:1752:MET:SD	2.59	0.42
1:B:1480:HIS:CD2	1:B:1486:LEU:HD23	2.37	0.42
1:B:1501:ASP:HA	1:B:1504:ILE:HB	2.01	0.42
1:B:1076:THR:HB	1:B:1080:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1677:GLU:HG3	1:B:1681:LYS:HD3	2.01	0.42
1:A:286:SER:HA	1:A:290:ILE:HD12	2.01	0.42
1:A:350:GLN:O	1:A:351:PHE:HB2	2.20	0.42
1:B:1083:LYS:HE3	1:B:1117:PHE:HD1	1.85	0.42
1:B:1343:THR:HG22	1:B:1348:VAL:O	2.20	0.42
1:B:1627:LEU:HB3	3:B:2094:HOH:O	2.19	0.42
1:B:1233:CYS:HB3	1:B:1235:ILE:H	1.85	0.41
1:B:1361:LYS:O	1:B:1365:MET:HB2	2.20	0.41
1:A:127:ASN:HB2	1:A:133:PHE:HE2	1.84	0.41
1:B:1180:THR:HB	1:B:1185:LEU:HG	2.01	0.41
1:B:1379:ASN:HD21	1:B:1382:VAL:HG21	1.85	0.41
1:A:288:ASP:O	1:A:292:LEU:HG	2.20	0.41
1:A:747:PRO:O	1:A:751:GLU:HG2	2.21	0.41
1:A:814:LYS:O	1:A:818:ILE:HG13	2.20	0.41
1:B:1222:ASP:HB3	1:B:1250:ARG:NH2	2.35	0.41
1:A:120:PRO:HD2	1:A:149:ILE:CD1	2.50	0.41
1:A:353:PRO:HA	1:A:354:PRO:HD2	1.84	0.41
1:A:730:ILE:HD12	1:A:730:ILE:HA	1.81	0.41
1:B:1094:LEU:O	1:B:1097:LEU:HD23	2.21	0.41
1:B:1773:ASP:O	1:B:1777:ILE:HB	2.21	0.41
1:A:652:HIS:HA	1:A:702:ILE:HD13	2.02	0.41
1:B:1282:ILE:CG2	1:B:1567:LEU:HD11	2.51	0.41
1:B:1611:LEU:HB3	1:B:1617:ALA:CB	2.50	0.41
1:A:301:ARG:HD3	1:A:304:SER:HA	2.01	0.41
1:B:1055:ILE:HG12	1:B:1056:ASP:H	1.86	0.41
1:B:1647:ILE:O	1:B:1651:VAL:HG23	2.21	0.41
1:B:1705:CYS:O	1:B:1709:VAL:HG23	2.20	0.41
1:A:192:PHE:HA	1:A:192:PHE:HD1	1.74	0.41
1:B:1677:GLU:HA	1:B:1681:LYS:HD3	2.03	0.41
1:B:1739:ARG:HH21	1:B:1742:PRO:HD3	1.86	0.41
1:A:389:PHE:CD2	1:A:391:PRO:HD3	2.56	0.41
1:B:1074:THR:HG21	1:B:1118:GLY:HA3	2.03	0.41
1:B:1578:ILE:HG21	1:B:1776:VAL:HG11	2.03	0.41
1:B:1585:PRO:HB2	1:B:1589:SER:HA	2.02	0.41
1:B:1752:MET:HA	1:B:1759:ALA:HB2	2.03	0.41
1:B:1716:HIS:CD2	1:B:1862:ILE:HG23	2.56	0.41
1:B:1400:TYR:O	1:B:1487:GLY:HA2	2.21	0.41
1:A:324:PRO:HG2	1:A:327:ILE:HG12	2.03	0.40
1:B:1212:TYR:HA	1:B:1241:ARG:O	2.22	0.40
1:B:1689:LYS:HA	1:B:1690:PRO:HD3	1.97	0.40
1:A:113:TRP:CE3	1:A:113:TRP:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:LYS:NZ	1:A:703:GLN:HG2	2.37	0.40
1:A:453:LYS:HD2	1:A:739:ARG:HA	2.02	0.40
1:A:739:ARG:NH2	1:A:742:PRO:HD3	2.36	0.40
1:A:822:ILE:CG2	1:A:845:LEU:HD13	2.46	0.40
1:B:1655:VAL:HG21	1:B:1702:ILE:CG1	2.51	0.40
1:B:1750:ASP:O	1:B:1753:VAL:HG12	2.21	0.40
1:B:1738:ARG:NH2	1:B:1762:ARG:HA	2.36	0.40
1:B:1068:MET:HA	1:B:1124:TYR:O	2.22	0.40
1:A:113:TRP:HZ3	1:A:117:PHE:HD1	1.69	0.40
1:A:304:SER:O	1:A:767:LYS:HD2	2.20	0.40
1:B:1265:ARG:C	1:B:1265:ARG:HE	2.24	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	831/864 (96%)	753 (91%)	58 (7%)	20 (2%)	7 7
1	B	831/864 (96%)	726 (87%)	77 (9%)	28 (3%)	4 3
All	All	1662/1728 (96%)	1479 (89%)	135 (8%)	48 (3%)	5 5

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	351	PHE
1	A	383	ILE
1	A	396	ASP
1	A	482	ASP
1	A	624	PRO
1	A	787	GLU

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Mol	Chain	Res	Type
1	A	853	LEU
1	B	1060	SER
1	B	1262	TYR
1	B	1265	ARG
1	B	1333	PRO
1	B	1449	LEU
1	B	1499	GLY
1	B	1621	PRO
1	B	1853	LEU
1	A	10	LYS
1	A	102	ALA
1	A	347	ASN
1	A	356	VAL
1	A	364	VAL
1	A	788	ILE
1	B	1160	PHE
1	B	1260	GLU
1	B	1264	PRO
1	B	1355	HIS
1	B	1482	ASP
1	B	1625	HIS
1	B	1723	GLN
1	A	299	GLN
1	A	318	GLU
1	B	1142	ASP
1	B	1192	PHE
1	B	1346	GLU
1	B	1365	MET
1	B	1500	VAL
1	A	99	THR
1	A	161	ARG
1	A	316	LEU
1	B	1484	ASP
1	B	1258	PRO
1	B	1030	SER
1	B	1624	PRO
1	A	101	GLY
1	B	1118	GLY
1	B	1363	GLY
1	B	1098	PRO
1	B	1364	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	730/750 (97%)	643 (88%)	87 (12%)	6	8
1	B	730/750 (97%)	644 (88%)	86 (12%)	6	8
All	All	1460/1500 (97%)	1287 (88%)	173 (12%)	6	8

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	23	LEU
1	A	70	LEU
1	A	76	THR
1	A	90	LEU
1	A	91	GLU
1	A	98	PRO
1	A	105	ASP
1	A	109	ILE
1	A	136	VAL
1	A	140	LEU
1	A	145	ASN
1	A	161	ARG
1	A	164	LYS
1	A	171	VAL
1	A	186	LYS
1	A	189	LYS
1	A	203	ARG
1	A	216	ASN
1	A	242	VAL
1	A	251	THR
1	A	267	GLU
1	A	272	LEU
1	A	275	SER
1	A	285	LEU
1	A	299	GLN
1	A	312	ASP

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	334	LEU
1	A	340	ILE
1	A	341	PHE
1	A	342	ARG
1	A	348	VAL
1	A	352	PRO
1	A	356	VAL
1	A	358	LYS
1	A	361	LYS
1	A	378	VAL
1	A	381	ASN
1	A	388	GLU
1	A	425	LEU
1	A	436	GLN
1	A	468	THR
1	A	470	LYS
1	A	480	HIS
1	A	482	ASP
1	A	485	ASN
1	A	494	LEU
1	A	505	TRP
1	A	532	VAL
1	A	545	SER
1	A	547	LEU
1	A	564	ILE
1	A	605	GLN
1	A	607	LEU
1	A	611	LEU
1	A	613	LYS
1	A	619	GLU
1	A	624	PRO
1	A	634	TYR
1	A	661	THR
1	A	667	GLN
1	A	669	THR
1	A	695	LYS
1	A	698	THR
1	A	700	ASP
1	A	703	GLN
1	A	715	LEU
1	A	725	PRO

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Mol	Chain	Res	Type
1	A	729	LEU
1	A	731	LEU
1	A	733	ARG
1	A	739	ARG
1	A	742	PRO
1	A	747	PRO
1	A	748	GLU
1	A	776	VAL
1	A	786	ASP
1	A	790	LEU
1	A	793	ARG
1	A	797	ASN
1	A	801	ASP
1	A	815	LEU
1	A	831	LEU
1	A	840	LEU
1	A	845	LEU
1	A	847	ARG
1	B	1020	LYS
1	B	1024	ASP
1	B	1059	THR
1	B	1062	LEU
1	B	1069	GLN
1	B	1075	GLN
1	B	1083	LYS
1	B	1096	THR
1	B	1103	ARG
1	B	1117	PHE
1	B	1127	ASN
1	B	1135	LEU
1	B	1139	LYS
1	B	1160	PHE
1	B	1181	PRO
1	B	1185	LEU
1	B	1191	GLU
1	B	1192	PHE
1	B	1195	LEU
1	B	1211	ASP
1	B	1238	TYR
1	B	1242	VAL
1	B	1257	LYS
1	B	1272	LEU

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Mol	Chain	Res	Type
1	B	1273	LYS
1	B	1278	LEU
1	B	1322	LYS
1	B	1338	LYS
1	B	1341	PHE
1	B	1346	GLU
1	B	1358	LYS
1	B	1361	LYS
1	B	1364	VAL
1	B	1381	ASN
1	B	1393	SER
1	B	1410	GLU
1	B	1414	ILE
1	B	1425	LEU
1	B	1468	THR
1	B	1485	ASN
1	B	1486	LEU
1	B	1503	THR
1	B	1505	TRP
1	B	1507	LEU
1	B	1517	SER
1	B	1522	LEU
1	B	1527	LEU
1	B	1529	THR
1	B	1532	VAL
1	B	1564	ILE
1	B	1570	GLN
1	B	1576	ASP
1	B	1587	LYS
1	B	1602	PHE
1	B	1607	LEU
1	B	1611	LEU
1	B	1620	ASP
1	B	1630	VAL
1	B	1632	GLU
1	B	1634	TYR
1	B	1641	LEU
1	B	1669	THR
1	B	1695	LYS
1	B	1703	GLN
1	B	1715	LEU
1	B	1723	GLN

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Mol	Chain	Res	Type
1	B	1733	ARG
1	B	1736	LEU
1	B	1748	GLU
1	B	1754	LYS
1	B	1777	ILE
1	B	1781	SER
1	B	1790	LEU
1	B	1793	ARG
1	B	1795	THR
1	B	1797	ASN
1	B	1801	ASP
1	B	1802	LYS
1	B	1809	LYS
1	B	1831	LEU
1	B	1832	ARG
1	B	1839	GLN
1	B	1847	ARG
1	B	1848	SER
1	B	1853	LEU
1	B	1856	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	166	ASN
1	A	216	ASN
1	A	347	ASN
1	A	381	ASN
1	A	411	GLN
1	A	511	HIS
1	A	528	ASN
1	A	541	ASN
1	A	557	HIS
1	A	563	ASN
1	A	625	HIS
1	A	666	GLN
1	A	672	GLN
1	A	683	HIS
1	A	703	GLN
1	A	723	GLN
1	A	732	ASN

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Mol	Chain	Res	Type
1	A	757	GLN
1	A	797	ASN
1	A	846	HIS
1	B	1075	GLN
1	B	1127	ASN
1	B	1166	ASN
1	B	1403	GLN
1	B	1428	GLN
1	B	1436	GLN
1	B	1480	HIS
1	B	1485	ASN
1	B	1528	ASN
1	B	1541	ASN
1	B	1565	ASN
1	B	1570	GLN
1	B	1683	HIS
1	B	1703	GLN
1	B	1720	ASN
1	B	1723	GLN
1	B	1797	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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.