



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:43 AM UTC

PDB ID : 5CSK / pdb_00005csk
Title : Crystal structure of yeast acetyl-CoA carboxylase, unbiotinylated
Authors : Wei, J.; Tong, L.
Deposited on : 2015-07-23
Resolution : 3.10 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
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

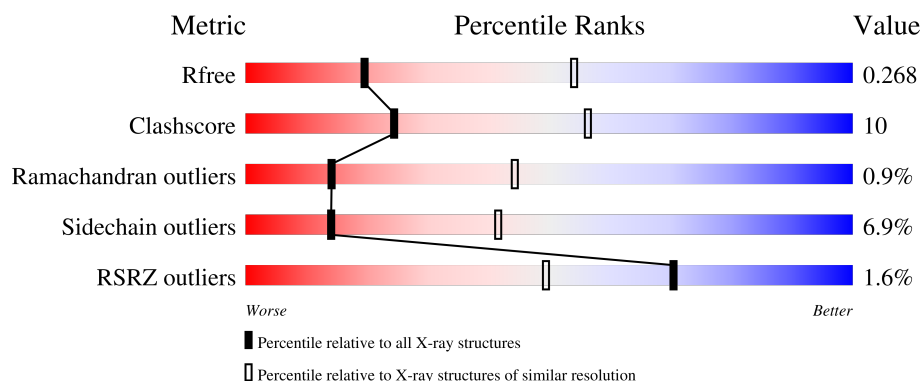
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	2218	0% 66% 22% 10%
1	B	2218	2% 67% 21% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31806 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1996	Total	C	N	O	S	0	0	0
			15828	10063	2733	2980	52			
1	B	2017	Total	C	N	O	S	0	0	0
			15978	10159	2758	3009	52			

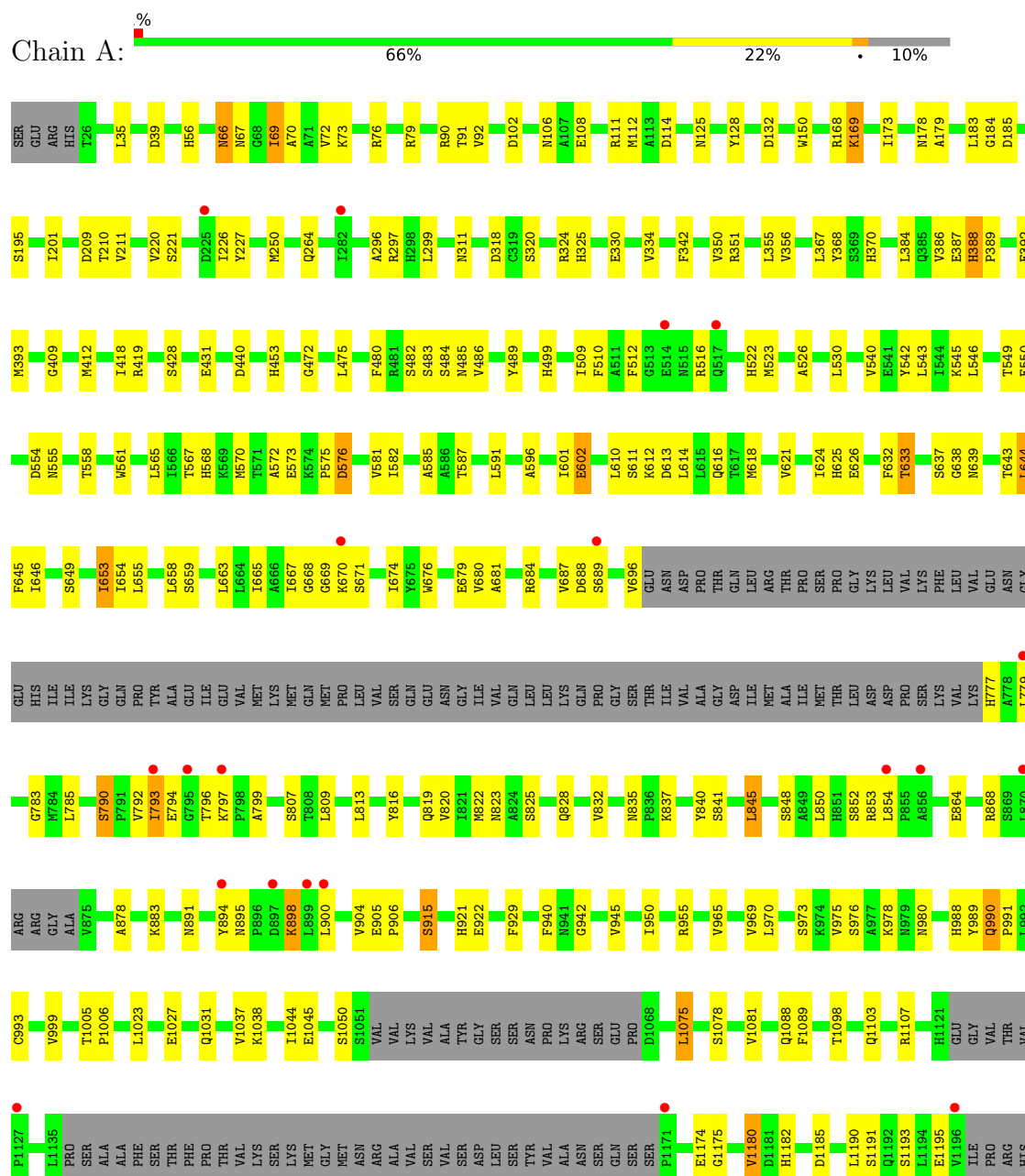
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	HIS	-	expression tag	UNP Q00955
A	2235	HIS	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
B	2234	HIS	-	expression tag	UNP Q00955
B	2235	HIS	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955

3 Residue-property plots [i](#)

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: Acetyl-CoA carboxylase



R2080	E1914	T1792	T1692	V1584	V1468	T1344	SER	L1135	Q990	L854	ASP
E2081	T1915	L1797	E1703	V1585	F1469	D1350	GLY	P1136	P991	L865	PRO
L2083	P1920	L1797	G1704	I1589	K1470	I1351	SER	S1137	S997	L868	THR
P2084	V1923	K1802	L1705	K1592	S1471	S1352	ALA	ALA	P1006	R868	GLN
L2085	W1924	M1807	A1714	I1593	S1477	I1353	SER	PHE	P1006	S889	ARG
L2089	H1925	S1807	Y1719	G1594	H1478	S1359	SER	SER	V1011	L870	THR
S2101	P1926	Y1809	Y1719	F1603	L1480	S1359	THR	THR	V1011	ARG	PRO
R2102	S1928	V1810	T1724	F1604	Y1487	M1365	PRO	PHE	E1012	GLY	PRO
R2103	E1943	K1813	I1725	N1605	Y1487	M1365	M1223	THR	E1014	A874	GLY
K2106	Q1944	V1818	C1730	K1606	K1490	I1368	V1224	VAL	S1015	V875	LYS
W2115	L1945	V1818	R1731	V1607	E1491	E1491	F1232	SER	R1026	F876	LEU
T2116	S1957	T1823	S1732	I1616	L1493	N1371	L1239	MET	I1030	P877	VAL
T2116	Q1960	D1825	I1735	I1619	R1497	V1374	R1241	MET	R1040	K883	VAL
A2118	R1961	T1825	G1736	K1824	Y1498	T1375	R1241	MET	R1040	D886	VAL
R2128	D1962	W1827	Y1738	A1632	K1499	D1376	R1243	ASN	I1044	D886	GLY
F1964	M1963	D1828	L1739	E1633	V1507	S1380	A1256	THR	V1052	D887	GLY
W2131	F1964	R1829	R1741	I1635	V1508	I1385	I1258	VAL	V1053	L899	HIS
R2138	D1980	F1833	L1742	V1636	Q1517	Q1517	I1261	ALA	Y1057	L900	ILE
H2141	Y1988	T1836	R1745	G1640	S1521	I1390	T1262	ASN	Q1058	V904	LYS
VAL	P1991	D1838	Q1748	V1641	F1537	F1407	F1278	SER	SER	E905	GLY
GLY	T1992	E1839	G1752	V1642	D1534	F1407	F1278	GLN	ASN	P906	GLN
GLU	V2001	T1840	G1751	W1643	T1533	G1406	P1273	SER	ASN	K913	PRO
A2146	A2022	Y1841	Q1752	G1648	D1534	F1407	P1273	LYS	LYS	Y914	ALA
T2152	G2093	D1842	Q1752	P1649	I1538	L1408	F1278	ARG	S1065	E921	GLY
S2162	L2025	V1843	A1759	D1650	S1539	E1409	Y1283	ILE	E794	H922	ILE
V2163	V2024	M1846	P1760	K1651	L1542	L1415	M1284	VAL	L1075	H923	VAL
D2164	P2027	G1849	I1762	G1652	E1543	F1653	E1285	MET	S1078	S924	MET
H2165	V2027	G1849	M1763	Q1654	E1544	S1422	E1286	MET	F926	F926	MET
D2168	V2031	T1852	M1765	Y1655	L1656	E1549	E1287	MET	V1081	H928	MET
R2169	G2032	G1855	L1766	V1657	L1550	K1430	Q1299	PRO	D1084	H928	PRO
Q2170	I2033	G1855	E1769	L1658	L1550	T1434	L1300	LEU	V806	Y933	LEU
R2034	F2035	Y1858	V1770	E1664	G1558	P1437	E1301	VAL	M822	F940	VAL
W2174	F2035	Y1858	Y1771	T1665	G1558	P1437	L1305	GLN	W675	N941	GLN
L2175	R2037	A1874	M1774	L1666	V1565	R1441	I1310	ASN	Q828	V945	ASN
E2176	S2059	K1875	L1775	K1667	A1566	F1567	I1317	GLY	V832	I950	GLY
E2177	ASN	V1878	Q1776	D1670	F1567	I1444	R1318	ILE	V832	I950	ILE
W2178	LYS	R1883	Q1776	V1681	K1568	I1445	R1318	VAL	N835	R955	VAL
L2180	LEU	I1887	I1782	I1682	V1570	V1451	V1322	GLN	P836	R955	GLN
T2181	LEU	P1888	I1782	I1682	V1570	V1451	V1322	LEU	L845	L967	LEU
L2182	ALA	P1888	I1782	I1682	V1570	V1451	V1322	LYS	L845	L967	LYS
D2183	PRO	V1894	M1783	M1683	T1573	T1454	D1333	GLN	V975	V975	GLN
L2186	GLU	V1894	M1786	F1688	T1573	T1454	D1333	VAL	S848	V975	VAL
L2189	H2068	V1984	G1787	V1689	V1460	K1461	T1338	THR	A849	V975	THR
L2190	E2068	V1984	G1787	V1689	V1460	K1461	T1338	VAL	L850	V975	VAL
W2192	F2076	M1909	V1739	I1690	E1466	E1466	I1341	GLY	H851	N979	GLY
ASN	F2076	M1909	V1739	V1593	E1466	E1466	I1341	THR	S852	N979	THR
THR	F2076	M1909	V1739	V1593	E1466	E1466	I1341	ASP	S852	L981	ASP
GLY	F2076	M1909	V1739	V1593	E1466	E1466	I1341	THR	S852	L981	THR
ASN	F2076	M1909	V1739	V1593	E1466	E1466	I1341	THR	S852	L981	ASN

L2191	
E2192	
S2193	
PHE	
ALA	
GLN	
ASP	
LEU	
ALA	
LYS	
ILE	
ARG	
SER	
ASP	
HIS	
ASP	
ASN	
ALA	
ILE	
ASP	
GLY	
LEU	
SER	
GLU	
VAL	
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LYS	
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THR	
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GLU	
LYS	
LEU	
LEU	
LYS	
THR	
LEU	
LYS	
HIS	
HIS	
HIS	
HIS	
HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.88Å 159.88Å 615.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.10 49.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.47-3.10) 93.3 (49.47-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.281 (Not available) , 0.268	Depositor DCC
R_{free} test set	6831 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31806	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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	0.77	1/16156 (0.0%)	1.02	34/21869 (0.2%)
1	B	0.77	1/16306 (0.0%)	1.02	32/22069 (0.1%)
All	All	0.77	2/32462 (0.0%)	1.02	66/43938 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1592	LYS	CA-C	-8.65	1.47	1.52
1	B	1573	THR	N-CA	5.40	1.49	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1990	PRO	CA-C-N	7.51	129.23	119.84
1	A	1990	PRO	C-N-CA	7.51	129.23	119.84
1	A	1174	GLU	N-CA-C	6.72	118.42	108.60
1	B	1571	VAL	CB-CA-C	-6.65	100.27	110.50
1	A	1434	THR	N-CA-C	6.60	118.56	111.36
1	A	1431	ASP	N-CA-C	-6.48	100.14	109.48
1	A	1770	VAL	N-CA-C	6.46	117.09	110.82
1	B	854	LEU	CA-C-N	6.45	126.40	119.76
1	B	854	LEU	C-N-CA	6.45	126.40	119.76
1	B	1894	VAL	N-CA-C	6.41	117.09	108.11
1	A	2152	ILE	CB-CA-C	-6.30	103.77	112.02
1	B	1740	VAL	N-CA-C	-6.04	104.62	110.72
1	A	1492	TRP	N-CA-C	-6.04	104.03	111.33
1	A	1927	ASN	N-CA-C	5.98	117.47	111.07
1	A	1078	SER	N-CA-C	-5.85	101.86	110.52
1	A	472	GLY	N-CA-C	-5.80	104.63	112.57
1	A	1508	VAL	CB-CA-C	-5.79	104.46	112.04
1	B	1810	VAL	CB-CA-C	-5.78	104.52	110.13
1	B	1479	HIS	N-CA-C	5.78	117.27	110.97
1	B	1585	VAL	CB-CA-C	-5.75	101.69	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1903	ILE	CB-CA-C	-5.68	105.65	110.94
1	B	1829	ARG	N-CA-C	5.56	114.54	108.14
1	A	388	HIS	CA-C-N	-5.54	114.11	119.87
1	A	388	HIS	C-N-CA	-5.54	114.11	119.87
1	A	1422	SER	N-CA-C	5.53	118.20	108.75
1	B	1508	VAL	CB-CA-C	-5.51	104.82	112.04
1	B	1487	TYR	CA-C-N	5.50	126.87	120.98
1	B	1487	TYR	C-N-CA	5.50	126.87	120.98
1	A	2089	ILE	N-CA-C	-5.48	105.16	110.42
1	A	1655	TYR	N-CA-C	5.47	115.06	107.73
1	B	1849	GLY	N-CA-C	-5.46	103.21	110.97
1	B	2152	ILE	CB-CA-C	-5.45	104.94	112.24
1	B	1487	TYR	N-CA-C	-5.43	101.52	109.50
1	A	1843	VAL	CB-CA-C	-5.42	102.40	111.29
1	B	143	VAL	N-CA-C	5.39	116.74	108.71
1	B	1497	ARG	CB-CA-C	-5.34	101.98	110.84
1	A	201	ILE	CA-C-N	5.33	126.50	119.84
1	A	201	ILE	C-N-CA	5.33	126.50	119.84
1	B	1810	VAL	N-CA-C	5.32	113.94	107.61
1	B	1044	ILE	N-CA-C	-5.30	105.54	110.53
1	B	2163	VAL	N-CA-C	5.30	116.38	108.54
1	B	832	VAL	CB-CA-C	-5.27	105.23	111.97
1	B	177	GLY	N-CA-C	5.23	118.97	112.64
1	A	840	TYR	N-CA-C	-5.22	105.48	111.07
1	B	1988	TYR	CA-C-N	-5.22	118.83	122.59
1	B	1988	TYR	C-N-CA	-5.22	118.83	122.59
1	B	1497	ARG	CG-CD-NE	-5.21	100.54	112.00
1	A	351	ARG	N-CA-C	-5.21	105.61	111.28
1	A	576	ASP	CA-C-N	-5.19	114.31	119.56
1	A	576	ASP	C-N-CA	-5.19	114.31	119.56
1	A	1571	VAL	CB-CA-C	-5.18	101.75	110.71
1	B	566	ILE	CB-CA-C	-5.17	105.36	111.97
1	B	1740	VAL	N-CA-CB	5.15	118.30	110.58
1	A	1493	LEU	N-CA-C	5.14	116.57	111.07
1	A	1735	ILE	CB-CA-C	-5.14	105.20	112.14
1	B	1493	LEU	CB-CA-C	-5.13	102.12	110.85
1	B	1923	VAL	N-CA-C	5.11	115.21	107.75
1	A	1282	ASN	N-CA-C	-5.11	102.72	110.28
1	A	1735	ILE	N-CA-CB	5.07	117.43	110.54
1	B	388	HIS	CA-C-N	-5.07	114.39	119.56
1	B	388	HIS	C-N-CA	-5.07	114.39	119.56
1	A	475	LEU	N-CA-C	-5.06	102.21	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1983	GLN	CA-C-N	-5.04	114.72	119.76
1	A	1983	GLN	C-N-CA	-5.04	114.72	119.76
1	A	69	ILE	CB-CA-C	-5.03	105.52	111.81
1	B	1797	LEU	N-CA-C	-5.01	105.73	111.14

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	15828	0	15783	316	1
1	B	15978	0	15941	344	0
All	All	31806	0	31724	630	1

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 10.

All (630) 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:1841:TYR:CE1	1:A:1846:MET:HE3	1.87	1.10
1:A:1835:PRO:HG3	1:A:1846:MET:HE2	1.30	1.09
1:A:1735:ILE:HD13	1:A:1735:ILE:H	1.19	1.07
1:B:941:ASN:HD21	1:B:1013:LEU:HA	1.31	0.92
1:B:1040:ARG:NH1	1:B:1081:VAL:O	2.02	0.92
1:A:1835:PRO:CG	1:A:1846:MET:HE2	1.99	0.92
1:A:1243:ARG:NH1	1:A:1283:TYR:O	2.02	0.91
1:A:587:THR:HG22	1:A:663:LEU:HD12	1.53	0.91
1:B:323:ARG:CZ	1:B:468:PHE:CE2	2.54	0.90
1:B:1135:LEU:HB3	1:B:1136:PRO:HD2	1.51	0.90
1:A:1431:ASP:OD2	1:A:1434:THR:OG1	1.93	0.86
1:B:1841:TYR:CE1	1:B:1846:MET:HE2	2.13	0.84
1:A:220:VAL:HG21	1:A:355:LEU:HG	1.60	0.83
1:B:587:THR:HG22	1:B:663:LEU:HD12	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ARG:NH2	1:B:123:THR:OG1	2.12	0.81
1:B:1841:TYR:HE1	1:B:1846:MET:HE2	1.47	0.79
1:A:945:VAL:HG11	1:A:950:ILE:HD11	1.63	0.79
1:A:296:ALA:HB3	1:A:367:LEU:HD11	1.65	0.78
1:A:1643:TRP:CE3	1:A:1649:PRO:HB2	2.18	0.78
1:A:2163:VAL:HA	1:A:2170:GLN:NE2	1.98	0.78
1:B:467:GLY:O	1:B:468:PHE:CD2	2.37	0.77
1:B:1766:LEU:HD12	1:B:1770:VAL:HG11	1.66	0.77
1:A:970:LEU:O	1:A:973:SER:OG	2.02	0.77
1:B:1317:ASN:HB3	1:B:1371:ASN:HD21	1.48	0.76
1:B:323:ARG:CZ	1:B:566:ILE:HG12	2.14	0.76
1:B:563:ASP:HA	1:B:566:ILE:HD12	1.68	0.76
1:A:69:ILE:HG23	1:A:489:TYR:CE1	2.21	0.74
1:B:319:CYS:SG	1:B:330:GLU:CD	2.70	0.74
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.68	0.73
1:B:822:MET:SD	1:B:981:LEU:HA	2.30	0.71
1:A:2004:ASP:OD2	1:A:2006:THR:HG22	1.88	0.71
1:B:124:ASN:HA	1:B:127:ASN:OD1	1.90	0.71
1:A:106:ASN:HD21	1:B:658:LEU:HB3	1.56	0.71
1:B:365:GLU:OE2	1:B:381:ASN:OD1	2.08	0.71
1:B:1084:ASP:HB3	1:B:1273:PRO:HD3	1.72	0.70
1:B:1444:ILE:HG23	1:B:1454:THR:HG22	1.73	0.70
1:A:545:LYS:HD2	1:A:572:ALA:O	1.92	0.70
1:A:1735:ILE:H	1:A:1735:ILE:CD1	1.99	0.70
1:A:330:GLU:OE2	1:A:387:GLU:HB3	1.93	0.69
1:A:1365:MET:HE1	1:A:1415:LEU:HD21	1.75	0.69
1:A:1735:ILE:HD13	1:A:1735:ILE:N	2.01	0.69
1:A:106:ASN:OD1	1:A:111:ARG:NH1	2.25	0.69
1:A:483:SER:HB3	1:A:486:VAL:HB	1.75	0.69
1:B:1135:LEU:HB3	1:B:1136:PRO:CD	2.23	0.69
1:A:72:VAL:HA	1:A:112:MET:HE1	1.75	0.68
1:B:1301:GLU:OE2	1:B:1441:ARG:NH2	2.23	0.67
1:B:2189:LEU:O	1:B:2193:SER:OG	2.10	0.67
1:B:1350:ASP:N	1:B:1350:ASP:OD1	2.27	0.67
1:B:2163:VAL:HA	1:B:2170:GLN:OE1	1.95	0.67
1:B:323:ARG:NH2	1:B:468:PHE:CE2	2.63	0.67
1:B:1653:PHE:H	1:B:1653:PHE:HD2	1.43	0.66
1:A:453:HIS:CD2	1:A:516:ARG:HA	2.30	0.66
1:A:1841:TYR:CE1	1:A:1846:MET:CE	2.74	0.66
1:A:2021:ARG:HD3	1:A:2095:ASP:OD2	1.96	0.65
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1317:ASN:HB3	1:B:1371:ASN:ND2	2.11	0.65
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.32	0.65
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.44	0.64
1:A:965:VAL:O	1:A:969:VAL:HG23	1.97	0.64
1:A:108:GLU:O	1:A:112:MET:HG3	1.97	0.64
1:B:453:HIS:CD2	1:B:516:ARG:HA	2.33	0.64
1:B:1081:VAL:HG13	1:B:1084:ASP:OD1	1.98	0.64
1:B:1078:SER:O	1:B:1108:ARG:NH2	2.31	0.63
1:A:611:SER:OG	1:A:612:LYS:N	2.25	0.63
1:A:1533:THR:OG1	1:A:1535:ASP:OD2	2.17	0.63
1:A:828:GLN:O	1:A:832:VAL:HG23	1.98	0.63
1:B:319:CYS:SG	1:B:330:GLU:OE2	2.57	0.63
1:B:323:ARG:NH2	1:B:468:PHE:HE2	1.97	0.63
1:A:1005:THR:HB	1:A:1006:PRO:HD3	1.81	0.63
1:B:387:GLU:OE2	1:B:458:ARG:NH2	2.32	0.63
1:A:1223:ASN:HB3	1:A:1262:THR:HB	1.79	0.63
1:B:955:ARG:NH1	1:B:1914:GLU:OE1	2.32	0.63
1:B:1770:VAL:HG13	1:B:1771:TYR:CD1	2.33	0.63
1:A:1593:ILE:HG22	1:A:1625:SER:OG	1.98	0.62
1:A:1972:SER:HB3	1:B:1742:LEU:HD13	1.79	0.62
1:A:485:ASN:HB3	1:A:512:PHE:HB3	1.82	0.62
1:B:101:GLU:HB3	1:B:499:HIS:CG	2.34	0.62
1:A:485:ASN:OD1	1:A:522:HIS:CD2	2.53	0.62
1:A:484:SER:OG	1:A:485:ASN:OD1	2.17	0.62
1:A:69:ILE:CG2	1:A:489:TYR:CE1	2.82	0.62
1:B:1222:ALA:O	1:B:1261:ILE:HA	1.99	0.62
1:A:368:TYR:OH	1:A:370:HIS:HD2	1.83	0.61
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.82	0.61
1:B:1730:CYS:HA	1:B:1752:GLN:OE1	2.01	0.61
1:A:324:ARG:O	1:A:325:HIS:HB2	1.99	0.61
1:A:211:VAL:HG13	1:A:220:VAL:HG13	1.83	0.61
1:A:102:ASP:OD1	1:A:499:HIS:NE2	2.32	0.61
1:B:900:LEU:O	1:B:904:VAL:HG22	2.01	0.60
1:A:2039:LYS:NZ	1:B:1633:GLU:OE1	2.33	0.60
1:A:2041:LEU:HD11	1:A:2051:TYR:OH	2.01	0.60
1:B:224:ASP:O	1:B:228:GLN:HG2	2.00	0.60
1:B:2174:TRP:O	1:B:2174:TRP:CE3	2.53	0.60
1:A:1783:MET:HE3	1:A:1788:VAL:HG11	1.84	0.60
1:A:945:VAL:CG1	1:A:950:ILE:HD11	2.31	0.60
1:B:1344:THR:HG21	1:B:1393:PHE:HZ	1.67	0.60
1:A:486:VAL:HG11	1:A:526:ALA:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.10	0.59
1:B:463:ASP:CG	1:B:537:ARG:HD2	2.27	0.59
1:A:132:ASP:HB2	1:B:848:SER:OG	2.02	0.59
1:B:905:GLU:HB3	1:B:906:PRO:HD3	1.85	0.59
1:B:1657:TYR:HB2	1:B:1688:PHE:O	2.02	0.59
1:B:2174:TRP:O	1:B:2174:TRP:CD2	2.55	0.59
1:A:568:HIS:O	1:A:570:MET:N	2.35	0.59
1:B:101:GLU:HB3	1:B:499:HIS:CD2	2.37	0.59
1:A:900:LEU:O	1:A:904:VAL:HG22	2.02	0.59
1:A:2041:LEU:CD1	1:A:2051:TYR:OH	2.50	0.59
1:A:1564:MET:CE	1:A:1585:VAL:HG12	2.33	0.58
1:A:1378:SER:HB3	1:A:1379:ASN:OD1	2.03	0.58
1:B:150:TRP:CE2	1:B:386:VAL:HB	2.38	0.58
1:A:679:GLU:OE2	1:A:684:ARG:NH1	2.37	0.58
1:B:583:CYS:SG	1:B:674:ILE:HD11	2.43	0.58
1:A:2044:MET:HE3	1:A:2082:LEU:HB2	1.84	0.58
1:A:1088:GLN:HG3	1:A:1268:LYS:HD3	1.86	0.58
1:B:654:ILE:HD12	1:B:792:VAL:HG23	1.86	0.58
1:A:895:ASN:CG	1:A:898:LYS:HA	2.28	0.58
1:A:2160:PRO:HB2	1:A:2162:SER:OG	2.03	0.58
1:B:1748:GLN:NE2	1:B:1789:SER:OG	2.37	0.58
1:B:1338:THR:HG21	1:B:1368:ILE:HG23	1.86	0.57
1:A:79:ARG:NH2	1:A:114:ASP:OD2	2.38	0.57
1:B:1466:GLU:O	1:B:1468:VAL:HG23	2.03	0.57
1:B:1843:VAL:HG21	1:B:1878:VAL:HG21	1.85	0.57
1:B:1593:ILE:CG2	1:B:1731:ARG:HH21	2.17	0.57
1:A:1182:HIS:HE1	1:A:1230:GLU:O	1.87	0.56
1:B:485:ASN:HB2	1:B:522:HIS:HD2	1.70	0.56
1:A:393:MET:HE1	1:A:512:PHE:HB2	1.87	0.56
1:A:1489:VAL:HG12	1:A:1490:LYS:H	1.70	0.56
1:A:1784:TYR:HH	1:A:1871:SER:HG	1.48	0.56
1:B:1580:ARG:NH2	1:B:1810:VAL:O	2.34	0.56
1:A:125:ASN:OD1	1:B:853:ARG:NH2	2.38	0.56
1:B:658:LEU:O	1:B:660:ASP:O	2.24	0.56
1:A:69:ILE:O	1:A:70:ALA:C	2.47	0.56
1:A:790:SER:OG	1:A:792:VAL:O	2.22	0.56
1:B:387:GLU:O	1:B:390:THR:OG1	2.18	0.56
1:A:975:VAL:O	1:A:976:SER:C	2.49	0.56
1:A:1827:TRP:O	1:A:1829:ARG:N	2.38	0.56
1:A:1842:ASP:O	1:A:1843:VAL:C	2.49	0.56
1:B:387:GLU:CD	1:B:458:ARG:HH21	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:TRP:CE2	1:B:565:LEU:HD11	2.40	0.56
1:A:848:SER:OG	1:B:132:ASP:HB2	2.06	0.55
1:B:799:ALA:O	1:B:803:LYS:HG3	2.06	0.55
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.88	0.55
1:A:297:ARG:NH2	1:A:555:ASN:O	2.40	0.55
1:B:205:GLY:O	1:B:208:VAL:HG23	2.06	0.55
1:B:1127:PRO:O	1:B:1128:ILE:HG13	2.06	0.55
1:B:2115:TRP:O	1:B:2118:ALA:N	2.36	0.55
1:A:1694:ILE:HA	1:B:2102:ARG:HD3	1.88	0.55
1:B:1406:GLY:HA2	1:B:1409:GLU:HG3	1.89	0.55
1:B:1766:LEU:HD12	1:B:1770:VAL:CG1	2.35	0.55
1:B:1770:VAL:HG13	1:B:1771:TYR:N	2.20	0.55
1:A:1658:LEU:HD13	1:A:1690:ILE:HD11	1.88	0.55
1:B:654:ILE:HD12	1:B:792:VAL:CG2	2.36	0.55
1:B:1305:LEU:HB3	1:B:1310:ILE:HD11	1.89	0.55
1:B:1406:GLY:HA2	1:B:1409:GLU:CG	2.36	0.55
1:B:2026:GLU:O	1:B:2027:PRO:C	2.50	0.55
1:A:637:SER:HA	1:A:816:TYR:HB3	1.89	0.55
1:B:1829:ARG:HB2	1:B:1830:PRO:HD2	1.89	0.55
1:B:1175:GLY:HA2	1:B:1221:VAL:O	2.07	0.55
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.04	0.54
1:B:130:ASN:OD1	1:B:130:ASN:C	2.50	0.54
1:B:1492:TRP:HZ3	1:B:1558:GLY:O	1.90	0.54
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.40	0.54
1:B:95:VAL:HG22	1:B:115:GLN:CG	2.37	0.54
1:A:582:ILE:HG23	1:A:653:ILE:HD11	1.89	0.54
1:B:323:ARG:CZ	1:B:468:PHE:HE2	2.16	0.54
1:A:1240:VAL:O	1:A:1243:ARG:HB2	2.07	0.54
1:B:668:GLY:H	1:B:791:PRO:HA	1.73	0.54
1:B:1422:SER:HB3	1:B:1445:ASN:OD1	2.07	0.54
1:A:601:ILE:O	1:A:602:GLU:C	2.51	0.54
1:A:679:GLU:OE2	1:A:684:ARG:HD2	2.07	0.54
1:A:318:ASP:OD1	1:A:320:SER:OG	2.24	0.53
1:A:1618:ARG:C	1:A:1619:ILE:HD12	2.33	0.53
1:A:1657:TYR:CD2	1:A:1687:ARG:HG2	2.43	0.53
1:B:1176:ILE:HG22	1:B:1178:MET:HE2	1.90	0.53
1:B:1592:LYS:C	1:B:1594:GLY:H	2.15	0.53
1:B:582:ILE:CG2	1:B:653:ILE:HD11	2.38	0.53
1:A:1365:MET:SD	1:A:1385:ILE:HD13	2.47	0.53
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.55	0.53
1:B:1469:PHE:O	1:B:1479:HIS:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LEU:N	1:A:644:LEU:HD23	2.24	0.53
1:B:2083:LEU:O	1:B:2084:PRO:C	2.51	0.53
1:A:296:ALA:HB1	1:A:368:TYR:O	2.09	0.53
1:A:2085:ILE:HG13	1:B:1650:ASP:HA	1.90	0.53
1:B:183:LEU:HD22	1:B:189:SER:OG	2.09	0.53
1:B:1344:THR:HG21	1:B:1393:PHE:CZ	2.43	0.53
1:A:1648:ASN:O	1:A:1650:ASP:N	2.41	0.53
1:B:56:HIS:CD2	1:B:409:GLY:HA3	2.44	0.53
1:A:618:MET:HE1	1:A:633:THR:OG1	2.08	0.53
1:A:1657:TYR:CE2	1:A:1687:ARG:HG2	2.44	0.53
1:A:1753:PRO:HB3	1:A:1775:LEU:HD23	1.90	0.53
1:B:663:LEU:HG	1:B:676:TRP:HZ3	1.74	0.53
1:A:106:ASN:ND2	1:B:658:LEU:HB3	2.22	0.53
1:B:319:CYS:HG	1:B:330:GLU:CD	2.17	0.53
1:B:545:LYS:O	1:B:549:THR:HG23	2.08	0.53
1:A:1631:MET:CE	1:B:2034:LYS:HB3	2.39	0.53
1:B:161:GLU:O	1:B:164:SER:OG	2.26	0.53
1:A:311:ASN:HB2	1:A:350:VAL:HG13	1.89	0.52
1:A:585:ALA:HA	1:A:621:VAL:HG11	1.91	0.52
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.24	0.52
1:A:482:SER:HB2	1:B:487:TRP:HB2	1.91	0.52
1:B:1751:GLY:HA2	1:B:1775:LEU:HD21	1.91	0.52
1:A:550:GLU:HG3	1:A:554:ASP:OD2	2.10	0.52
1:B:584:GLY:HA2	1:B:685:LEU:HD11	1.90	0.52
1:B:1084:ASP:OD1	1:B:1084:ASP:N	2.39	0.52
1:B:1178:MET:HE3	1:B:1224:VAL:HG22	1.91	0.52
1:B:1827:TRP:O	1:B:1829:ARG:N	2.42	0.52
1:A:67:ASN:ND2	1:A:128:TYR:CE2	2.77	0.52
1:A:90:ARG:O	1:A:91:THR:C	2.52	0.52
1:A:864:GLU:OE1	1:A:868:ARG:NH1	2.43	0.52
1:A:1691:LYS:HA	1:A:1691:LYS:HE2	1.91	0.52
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.57	0.52
1:A:56:HIS:CD2	1:A:409:GLY:HA3	2.44	0.52
1:A:297:ARG:HD2	1:A:320:SER:OG	2.10	0.52
1:B:1243:ARG:NH1	1:B:1283:TYR:O	2.42	0.52
1:B:1593:ILE:O	1:B:1593:ILE:HG22	2.10	0.52
1:B:1762:ILE:O	1:B:1765:MET:HB2	2.10	0.52
1:B:990:GLN:HG3	1:B:991:PRO:N	2.25	0.52
1:A:480:PHE:HD1	1:A:530:LEU:HD13	1.75	0.52
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	1.91	0.52
1:B:1759:ALA:H	1:B:1774:ASN:ND2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:THR:HG23	1:A:645:PHE:HB2	1.91	0.51
1:B:682:ALA:HB1	1:B:694:LEU:O	2.10	0.51
1:A:1256:ALA:O	1:A:1257:SER:C	2.52	0.51
1:B:1369:LEU:HD21	1:B:1415:LEU:HD23	1.91	0.51
1:A:66:ASN:HD22	1:A:67:ASN:H	1.56	0.51
1:A:1516:ARG:HG2	1:A:1537:PHE:CG	2.46	0.51
1:A:581:VAL:HG12	1:A:632:PHE:CZ	2.45	0.51
1:A:1709:GLY:O	1:A:1710:LEU:C	2.52	0.51
1:A:1841:TYR:HE1	1:A:1846:MET:HE3	1.67	0.51
1:B:2183:ASP:HA	1:B:2186:LEU:HD12	1.92	0.51
1:A:220:VAL:CG2	1:A:355:LEU:HG	2.37	0.51
1:A:613:ASP:O	1:A:616:GLN:HB2	2.11	0.51
1:A:1493:LEU:HD11	1:A:1507:TYR:CE1	2.45	0.51
1:A:1727:LEU:HD12	1:A:1747:ILE:O	2.10	0.51
1:B:47:ARG:O	1:B:50:VAL:N	2.44	0.51
1:B:646:ILE:HG22	1:B:649:SER:OG	2.11	0.51
1:A:1315:THR:O	1:A:1317:ASN:N	2.43	0.51
1:B:1333:ASP:OD2	1:B:1490:LYS:HB2	2.10	0.51
1:A:822:MET:HE3	1:A:823:ASN:OD1	2.11	0.51
1:B:475:LEU:O	1:B:494:ASN:O	2.28	0.51
1:A:942:GLY:HA3	1:A:945:VAL:HG23	1.93	0.51
1:B:1827:TRP:CE3	1:B:1828:ASP:HA	2.46	0.51
1:A:1338:THR:HG21	1:A:1368:ILE:HG23	1.93	0.50
1:A:1353:ILE:HD12	1:A:1394:ASP:O	2.11	0.50
1:A:1404:PHE:O	1:A:1407:PHE:N	2.44	0.50
1:A:2101:SER:HB2	1:B:1692:THR:HG21	1.93	0.50
1:B:1909:ASN:C	1:B:1909:ASN:HD22	2.18	0.50
1:A:211:VAL:CG1	1:A:220:VAL:HG13	2.41	0.50
1:B:1497:ARG:O	1:B:1498:TYR:C	2.50	0.50
1:A:591:LEU:HD21	1:A:676:TRP:CZ2	2.47	0.50
1:A:668:GLY:HA2	1:A:790:SER:O	2.12	0.50
1:B:1223:ASN:HB3	1:B:1262:THR:HB	1.93	0.50
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.12	0.50
1:B:147:TRP:CH2	1:B:149:GLY:HA3	2.47	0.50
1:B:925:ILE:O	1:B:928:HIS:HB3	2.11	0.50
1:B:386:VAL:CG1	1:B:458:ARG:NH2	2.75	0.50
1:B:940:PHE:HA	1:B:950:ILE:HD13	1.92	0.50
1:B:1763:ASN:OD1	1:B:1770:VAL:HG12	2.12	0.50
1:A:940:PHE:HA	1:A:950:ILE:HD13	1.92	0.50
1:A:970:LEU:HA	1:A:973:SER:OG	2.12	0.50
1:B:561:TRP:CZ2	1:B:565:LEU:HD11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1616:ILE:HD12	1:B:1813:LYS:HB3	1.92	0.50
1:B:2033:ILE:O	1:B:2034:LYS:HD2	2.12	0.50
1:A:1643:TRP:CE3	1:A:1649:PRO:CB	2.94	0.50
1:A:1708:SER:CB	1:B:2001:VAL:HG12	2.42	0.50
1:B:1451:VAL:HG22	1:B:1517:GLN:HG2	1.94	0.50
1:B:1633:GLU:HA	1:B:1636:VAL:CG2	2.41	0.50
1:B:2022:ALA:HB3	1:B:2103:MET:HE2	1.94	0.50
1:B:323:ARG:NH2	1:B:566:ILE:HG23	2.26	0.49
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.77	0.49
1:B:1592:LYS:C	1:B:1594:GLY:N	2.70	0.49
1:A:393:MET:CE	1:A:512:PHE:HB2	2.42	0.49
1:A:1589:ILE:O	1:A:1589:ILE:HG13	2.12	0.49
1:B:377:PHE:CZ	1:B:379:GLU:HA	2.47	0.49
1:B:1352:SER:O	1:B:1353:ILE:C	2.54	0.49
1:B:1371:ASN:O	1:B:1375:THR:HG23	2.11	0.49
1:A:794:GLU:OE1	1:A:794:GLU:N	2.32	0.49
1:B:1493:LEU:HD11	1:B:1557:PRO:HB2	1.93	0.49
1:A:486:VAL:HG11	1:A:526:ALA:HB2	1.94	0.49
1:A:669:GLY:O	1:B:115:GLN:HB3	2.12	0.49
1:B:486:VAL:HG11	1:B:526:ALA:CB	2.43	0.49
1:B:1603:PHE:O	1:B:1607:VAL:HG23	2.13	0.49
1:A:108:GLU:HG2	1:A:111:ARG:NH2	2.28	0.49
1:B:1593:ILE:CG2	1:B:1731:ARG:NH2	2.76	0.49
1:B:363:THR:HG21	1:B:385:GLN:OE1	2.13	0.49
1:B:1762:ILE:HG21	1:B:1771:TYR:HE1	1.77	0.49
1:B:2086:TYR:HA	1:B:2089:ILE:HD12	1.94	0.49
1:A:904:VAL:O	1:A:905:GLU:C	2.56	0.49
1:A:2044:MET:HE1	1:A:2079:GLU:HA	1.95	0.49
1:B:1272:TYR:CD1	1:B:1318:ARG:HD2	2.47	0.49
1:A:2004:ASP:OD2	1:A:2006:THR:CG2	2.60	0.49
1:B:323:ARG:NH2	1:B:566:ILE:HG12	2.27	0.49
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.78	0.49
1:A:1781:GLN:H	1:A:1781:GLN:CD	2.21	0.48
1:A:644:LEU:HD21	1:A:653:ILE:HD12	1.95	0.48
1:A:1582:PHE:CD2	1:A:1807:MET:HE1	2.48	0.48
1:A:2047:LEU:HD13	1:B:1641:VAL:HG23	1.94	0.48
1:B:630:TYR:CE1	1:B:781:PHE:CD1	3.01	0.48
1:B:850:LEU:O	1:B:851:HIS:C	2.55	0.48
1:A:1373:GLU:OE2	1:A:1414:ARG:NH2	2.42	0.48
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.13	0.48
1:A:2164:ASP:O	1:A:2165:HIS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:GLN:O	1:A:1107:ARG:CG	2.61	0.48
1:A:1222:ALA:O	1:A:1261:ILE:HA	2.13	0.48
1:A:1779:GLY:HA3	1:A:1781:GLN:HE22	1.78	0.48
1:B:927:VAL:HG13	1:B:1006:PRO:HG3	1.95	0.48
1:B:341:THR:HG21	1:B:368:TYR:HE1	1.78	0.48
1:B:1095:PRO:HA	1:B:1098:THR:HB	1.95	0.48
1:A:73:LYS:HE3	1:A:389:PRO:HG3	1.95	0.48
1:B:1408:LEU:HD22	1:B:1415:LEU:CD1	2.44	0.48
1:B:1925:HIS:H	1:B:1928:SER:HB3	1.77	0.48
1:B:865:LEU:HD12	1:B:868:ARG:NH2	2.28	0.48
1:A:582:ILE:CG2	1:A:653:ILE:HD11	2.44	0.48
1:A:1772:THR:N	1:A:1776:GLN:OE1	2.44	0.48
1:B:150:TRP:CZ2	1:B:386:VAL:HG23	2.49	0.48
1:B:1648:ASN:O	1:B:1651:LYS:HB2	2.13	0.48
1:A:485:ASN:OD1	1:A:522:HIS:NE2	2.47	0.48
1:B:1422:SER:CB	1:B:1445:ASN:OD1	2.61	0.48
1:A:654:ILE:HD12	1:A:792:VAL:CG2	2.43	0.47
1:B:684:ARG:CB	1:B:684:ARG:HH11	2.26	0.47
1:B:1766:LEU:CD1	1:B:1770:VAL:HG11	2.41	0.47
1:B:1829:ARG:NH1	1:B:1858:TYR:HB3	2.29	0.47
1:A:565:LEU:O	1:A:568:HIS:O	2.31	0.47
1:A:2044:MET:HE3	1:A:2082:LEU:CB	2.44	0.47
1:B:102:ASP:OD1	1:B:499:HIS:HE1	1.97	0.47
1:A:655:LEU:HD22	1:A:663:LEU:HD22	1.95	0.47
1:A:1576:TYR:CE1	1:A:1819:PRO:HB3	2.49	0.47
1:B:386:VAL:HG13	1:B:458:ARG:NH2	2.29	0.47
1:B:1643:TRP:CD1	1:B:1643:TRP:H	2.31	0.47
1:A:72:VAL:HA	1:A:112:MET:CE	2.43	0.47
1:A:575:PRO:O	1:A:576:ASP:C	2.58	0.47
1:B:405:GLN:HA	1:B:408:MET:HE3	1.97	0.47
1:B:1180:VAL:CG1	1:B:1185:ASP:HB2	2.44	0.47
1:B:1544:GLU:OE1	1:B:1606:LYS:NZ	2.36	0.47
1:A:178:ASN:OD1	1:A:179:ALA:N	2.48	0.47
1:A:687:VAL:HG12	1:A:688:ASP:OD2	2.15	0.47
1:A:1350:ASP:OD1	1:A:1350:ASP:N	2.48	0.47
1:A:1633:GLU:HA	1:A:1636:VAL:HG23	1.97	0.47
1:B:322:GLN:O	1:B:562:LEU:HB3	2.14	0.47
1:B:1030:ILE:HD13	1:B:1371:ASN:OD1	2.14	0.47
1:B:1278:PHE:CE1	1:B:1285:GLU:HB2	2.50	0.47
1:B:1408:LEU:HD12	1:B:1444:ILE:HG22	1.97	0.47
1:B:1582:PHE:CD2	1:B:1807:MET:HE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:HD23	1:A:540:VAL:HG11	1.97	0.47
1:A:558:THR:H	1:A:561:TRP:HB2	1.78	0.47
1:A:1180:VAL:HG13	1:A:1185:ASP:HB2	1.97	0.47
1:B:1632:ALA:HB1	1:B:1634:GLU:OE1	2.15	0.47
1:A:220:VAL:HG12	1:A:221:SER:N	2.30	0.47
1:A:250:MET:SD	1:A:264:GLN:HG2	2.54	0.47
1:A:1404:PHE:O	1:A:1405:GLY:C	2.57	0.47
1:A:150:TRP:CZ2	1:A:386:VAL:HG23	2.50	0.46
1:A:480:PHE:HZ	1:A:486:VAL:HG12	1.80	0.46
1:A:1736:GLY:O	1:A:1740:VAL:HG23	2.15	0.46
1:B:46:LEU:O	1:B:50:VAL:HG23	2.15	0.46
1:B:618:MET:HE1	1:B:633:THR:OG1	2.14	0.46
1:A:1631:MET:HE3	1:B:2034:LYS:HB3	1.96	0.46
1:B:1258:ILE:O	1:B:1258:ILE:HG22	2.15	0.46
1:B:1365:MET:SD	1:B:1385:ILE:HD13	2.55	0.46
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.15	0.46
1:A:1223:ASN:HB2	1:A:1264:MET:HE2	1.97	0.46
1:B:211:VAL:HG11	1:B:220:VAL:CG1	2.45	0.46
1:B:1408:LEU:HD22	1:B:1415:LEU:HD11	1.96	0.46
1:B:2036:ARG:O	1:B:2037:ARG:C	2.57	0.46
1:A:1981:TYR:CD2	1:A:1985:ILE:HD11	2.50	0.46
1:B:163:LEU:O	1:B:166:SER:HB3	2.14	0.46
1:B:1197:ILE:HD13	1:B:1256:ALA:HA	1.97	0.46
1:B:1770:VAL:CG1	1:B:1771:TYR:N	2.79	0.46
1:A:389:PRO:HB2	1:A:510:PHE:CE1	2.51	0.46
1:B:2022:ALA:HB3	1:B:2103:MET:CE	2.46	0.46
1:A:646:ILE:HG21	1:A:785:LEU:HG	1.97	0.46
1:A:1587:ASN:ND2	1:A:1620:TYR:OH	2.48	0.46
1:B:644:LEU:O	1:B:650:LYS:HA	2.15	0.46
1:B:1180:VAL:HG13	1:B:1185:ASP:HB2	1.98	0.46
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.96	0.46
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.16	0.46
1:A:76:ARG:HD3	1:B:529:GLU:OE2	2.15	0.46
1:A:891:ASN:HB3	1:A:894:TYR:HB2	1.97	0.46
1:A:1479:HIS:ND1	1:A:1480:LEU:HG	2.30	0.46
1:A:1571:VAL:O	1:A:1579:GLY:HA2	2.15	0.46
1:A:1652:GLY:HA2	1:B:2085:ILE:HD11	1.98	0.46
1:B:1639:PHE:CD1	1:B:1639:PHE:C	2.93	0.46
1:B:1732:SER:OG	1:B:1736:GLY:C	2.59	0.46
1:A:368:TYR:OH	1:A:370:HIS:CD2	2.68	0.46
1:A:1427:ILE:HG22	1:A:1428:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1825:ASP:C	1:B:1825:ASP:OD2	2.59	0.46
1:A:90:ARG:C	1:A:92:VAL:N	2.72	0.46
1:A:850:LEU:O	1:A:854:LEU:HG	2.16	0.46
1:B:301:VAL:CG1	1:B:313:SER:HB2	2.46	0.46
1:B:498:ILE:HD12	1:B:536:PHE:CE2	2.51	0.46
1:B:1317:ASN:CB	1:B:1371:ASN:HD21	2.25	0.46
1:B:1592:LYS:O	1:B:1594:GLY:N	2.49	0.46
1:A:183:LEU:HD21	1:A:356:VAL:HG11	1.99	0.45
1:A:1987:ILE:HG21	1:A:2014:MET:HE2	1.98	0.45
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.97	0.45
1:A:1443:LEU:HD12	1:A:1443:LEU:N	2.31	0.45
1:B:646:ILE:HG23	1:B:647:ASN:N	2.31	0.45
1:B:1492:TRP:CZ3	1:B:1558:GLY:O	2.69	0.45
1:B:1493:LEU:HD21	1:B:1558:GLY:HA3	1.97	0.45
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.17	0.45
1:B:2115:TRP:O	1:B:2116:THR:C	2.58	0.45
1:B:646:ILE:CG2	1:B:649:SER:OG	2.64	0.45
1:B:2079:GLU:C	1:B:2081:GLU:H	2.25	0.45
1:A:905:GLU:HB3	1:A:906:PRO:HD3	1.97	0.45
1:A:993:CYS:SG	1:A:999:VAL:HG12	2.56	0.45
1:B:306:ASP:OD1	1:B:310:THR:HB	2.17	0.45
1:B:458:ARG:O	1:B:543:LEU:HD11	2.16	0.45
1:A:299:LEU:HD13	1:A:334:VAL:HG11	1.97	0.45
1:A:1692:THR:HG21	1:B:2101:SER:HB2	1.99	0.45
1:B:55:GLY:HA2	1:B:409:GLY:O	2.16	0.45
1:B:1657:TYR:HA	1:B:1690:ILE:HG12	1.99	0.45
1:A:485:ASN:HB2	1:A:522:HIS:HD2	1.80	0.45
1:A:667:ILE:HG22	1:A:667:ILE:O	2.15	0.45
1:A:988:HIS:HD2	1:A:989:TYR:CD2	2.34	0.45
1:B:1374:VAL:O	1:B:1374:VAL:HG12	2.16	0.45
1:B:1593:ILE:HG22	1:B:1731:ARG:HH21	1.81	0.45
1:A:1827:TRP:CE3	1:A:1828:ASP:HA	2.52	0.45
1:B:35:LEU:HD23	1:B:169:LYS:HD2	1.99	0.45
1:B:822:MET:SD	1:B:981:LEU:CA	3.04	0.45
1:B:1783:MET:HE3	1:B:1788:VAL:CB	2.46	0.45
1:A:132:ASP:CB	1:B:848:SER:OG	2.64	0.45
1:A:419:ARG:CZ	1:A:428:SER:O	2.65	0.45
1:B:1808:SER:OG	1:B:1883:ARG:NH2	2.50	0.45
1:A:482:SER:HB3	1:B:482:SER:HB3	1.98	0.45
1:A:2154:ARG:O	1:A:2157:SER:OG	2.32	0.45
1:B:150:TRP:NE1	1:B:386:VAL:HB	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2131:ASN:HB3	1:B:2175:ILE:HG21	1.99	0.45
1:A:1344:THR:HG21	1:A:1393:PHE:HZ	1.82	0.45
1:B:1376:ASP:OD1	1:B:1376:ASP:C	2.59	0.45
1:A:509:ILE:HG22	1:A:523:MET:HE1	1.99	0.44
1:A:1045:GLU:HG3	1:A:1089:PHE:CE1	2.52	0.44
1:B:480:PHE:HD1	1:B:530:LEU:HD13	1.83	0.44
1:A:210:THR:O	1:A:226:ILE:HG21	2.17	0.44
1:B:1135:LEU:HD23	1:B:1135:LEU:HA	1.85	0.44
1:A:1175:GLY:HA2	1:A:1221:VAL:O	2.17	0.44
1:A:1757:THR:HG22	1:A:1762:ILE:HG13	1.98	0.44
1:A:793:ILE:HD13	1:B:117:ILE:HD11	2.00	0.44
1:A:809:LEU:HD12	1:A:929:PHE:CE2	2.53	0.44
1:A:1344:THR:HG21	1:A:1393:PHE:CZ	2.52	0.44
1:A:1384:HIS:CD2	1:A:1385:ILE:N	2.86	0.44
1:A:1786:ASN:OD1	1:B:1964:PHE:O	2.35	0.44
1:B:79:ARG:HG2	1:B:89:ASP:O	2.17	0.44
1:B:800:TYR:O	1:B:801:LYS:C	2.61	0.44
1:B:1081:VAL:CG1	1:B:1084:ASP:OD1	2.66	0.44
1:B:1272:TYR:CE1	1:B:1318:ARG:HD2	2.52	0.44
1:B:1649:PRO:C	1:B:1651:LYS:H	2.24	0.44
1:B:1770:VAL:CG1	1:B:1771:TYR:CD1	3.00	0.44
1:A:1027:GLU:O	1:A:1031:GLN:HG3	2.17	0.44
1:A:1619:ILE:HD12	1:A:1619:ILE:N	2.32	0.44
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.17	0.44
1:A:2005:PRO:HA	1:A:2012:MET:HE2	1.99	0.44
1:B:1783:MET:HE3	1:B:1788:VAL:HB	2.00	0.44
1:B:668:GLY:HA2	1:B:790:SER:O	2.17	0.44
1:B:1823:THR:O	1:B:1824:LYS:C	2.59	0.44
1:A:1701:GLY:HA2	1:B:2024:VAL:HG23	2.00	0.44
1:A:2147:SER:O	1:A:2148:ARG:C	2.61	0.44
1:B:876:PHE:O	1:B:878:ALA:N	2.50	0.44
1:B:480:PHE:HZ	1:B:486:VAL:HG12	1.82	0.44
1:B:1460:VAL:HG12	1:B:1461:LYS:N	2.31	0.44
1:B:2141:HIS:O	1:B:2190:LYS:NZ	2.50	0.44
1:A:638:GLY:O	1:A:639:ASN:C	2.61	0.43
1:A:1756:LEU:HD23	1:B:1963:MET:SD	2.58	0.43
1:B:304:LEU:HD11	1:B:406:ILE:CD1	2.48	0.43
1:B:388:HIS:N	1:B:389:PRO:CD	2.81	0.43
1:A:1037:VAL:O	1:A:1038:LYS:C	2.60	0.43
1:A:1432:PRO:HG2	1:A:1433:GLN:H	1.83	0.43
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1580:ARG:HG3	1:B:1580:ARG:HH11	1.83	0.43
1:A:546:LEU:O	1:A:549:THR:OG1	2.31	0.43
1:A:1444:ILE:HG23	1:A:1454:THR:HG22	1.99	0.43
1:A:1708:SER:HB2	1:B:2001:VAL:HG12	2.00	0.43
1:A:2128:ARG:HG3	1:A:2168:ASP:HA	2.01	0.43
1:B:1833:PHE:C	1:B:1833:PHE:CD2	2.96	0.43
1:B:2116:THR:HG22	1:B:2117:GLU:OE2	2.18	0.43
1:A:624:ILE:HD12	1:A:696:VAL:C	2.43	0.43
1:A:1075:LEU:HD12	1:A:1075:LEU:HA	1.91	0.43
1:A:1995:LEU:HD12	1:A:1995:LEU:HA	1.85	0.43
1:B:1341:ILE:HG23	1:B:1390:ILE:HD12	2.00	0.43
1:B:1479:HIS:ND1	1:B:1480:LEU:HG	2.34	0.43
1:B:1703:GLU:OE1	1:B:1703:GLU:N	2.37	0.43
1:B:1843:VAL:CG2	1:B:1878:VAL:HG21	2.48	0.43
1:B:2164:ASP:O	1:B:2165:HIS:C	2.61	0.43
1:A:1766:LEU:HD12	1:A:1770:VAL:HG21	2.01	0.43
1:B:681:ALA:O	1:B:696:VAL:HG23	2.17	0.43
1:A:542:TYR:O	1:A:543:LEU:C	2.61	0.43
1:A:665:ILE:HD12	1:A:674:ILE:CD1	2.49	0.43
1:B:462:GLU:O	1:B:464:PRO:HD3	2.19	0.43
1:B:913:LYS:HD2	1:B:914:TYR:CE2	2.52	0.43
1:B:1374:VAL:O	1:B:1374:VAL:CG1	2.66	0.43
1:B:389:PRO:HA	1:B:392:GLU:HB2	2.01	0.43
1:B:835:ASN:C	1:B:835:ASN:ND2	2.76	0.43
1:B:921:HIS:O	1:B:922:GLU:C	2.61	0.43
1:B:1638:LEU:O	1:B:1658:LEU:HD22	2.18	0.43
1:B:1943:GLU:O	1:B:1944:GLN:C	2.61	0.43
1:A:681:ALA:O	1:A:696:VAL:HG23	2.19	0.43
1:A:942:GLY:HA3	1:A:945:VAL:CG2	2.48	0.43
1:A:1636:VAL:HB	1:A:1637:PRO:HD3	2.01	0.43
1:B:386:VAL:HG13	1:B:458:ARG:HH21	1.84	0.43
1:B:306:ASP:HA	1:B:406:ILE:HG23	2.01	0.43
1:A:195:SER:HA	1:A:209:ASP:HB2	2.01	0.43
1:A:1249:ASN:O	1:A:1250:LYS:C	2.61	0.43
1:B:131:VAL:HG13	1:B:159:LEU:HA	2.00	0.43
1:B:186:LYS:O	1:B:190:THR:OG1	2.34	0.43
1:B:640:ASP:OD1	1:B:640:ASP:N	2.52	0.43
1:B:828:GLN:O	1:B:832:VAL:HG23	2.19	0.43
1:B:941:ASN:ND2	1:B:1013:LEU:HA	2.14	0.43
1:A:878:ALA:HB3	1:A:915:SER:HA	2.01	0.42
1:B:1655:TYR:CD1	1:B:1689:VAL:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:ARG:O	1:A:1744:GLN:N	2.51	0.42
1:B:634:VAL:HG13	1:B:644:LEU:CD2	2.49	0.42
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.33	0.42
1:B:1852:THR:HB	1:B:1855:GLY:O	2.19	0.42
1:A:813:LEU:HA	1:A:978:LYS:HG2	2.01	0.42
1:A:1304:ARG:C	1:A:1306:SER:H	2.27	0.42
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.19	0.42
1:A:1808:SER:O	1:A:1883:ARG:NH2	2.52	0.42
1:B:124:ASN:N	1:B:124:ASN:HD22	2.18	0.42
1:B:624:ILE:HG12	1:B:629:ARG:HB2	2.00	0.42
1:B:1299:GLN:O	1:B:1388:ASN:ND2	2.47	0.42
1:B:1285:GLU:HG2	1:B:1287:GLU:HG2	2.01	0.42
1:B:1581:GLN:HB2	1:B:1616:ILE:HD11	2.00	0.42
1:B:1836:THR:HB	1:B:1839:GLU:HB2	2.00	0.42
1:A:384:LEU:HD11	1:A:388:HIS:CG	2.54	0.42
1:A:970:LEU:C	1:A:973:SER:OG	2.62	0.42
1:A:1408:LEU:CD1	1:A:1444:ILE:HG22	2.49	0.42
1:B:73:LYS:NZ	1:B:77:SER:OG	2.42	0.42
1:B:781:PHE:CE2	1:B:783:GLY:O	2.73	0.42
1:B:1406:GLY:HA2	1:B:1409:GLU:HG2	2.02	0.42
1:B:1782:ILE:O	1:B:1786:ASN:HB2	2.19	0.42
1:A:921:HIS:O	1:A:922:GLU:C	2.62	0.42
1:B:556:THR:C	1:B:557:ILE:HG13	2.45	0.42
1:B:1365:MET:O	1:B:1369:LEU:HG	2.19	0.42
1:A:173:ILE:O	1:A:173:ILE:HG22	2.19	0.42
1:A:1639:PHE:CD1	1:A:1639:PHE:C	2.97	0.42
1:A:2159:TYR:CE1	1:A:2171:VAL:HG13	2.55	0.42
1:B:1286:ASN:C	1:B:1286:ASN:OD1	2.62	0.42
1:B:1670:ASP:OD1	1:B:1670:ASP:O	2.37	0.42
1:A:835:ASN:OD1	1:A:837:LYS:HB2	2.20	0.42
1:A:990:GLN:HG3	1:A:991:PRO:CD	2.50	0.42
1:A:1408:LEU:HD12	1:A:1444:ILE:HG22	2.02	0.42
1:A:1593:ILE:HG22	1:A:1593:ILE:O	2.20	0.42
1:A:1874:ALA:HB2	1:A:1927:ASN:HB2	2.02	0.42
1:B:368:TYR:CE2	1:B:370:HIS:HA	2.55	0.42
1:B:1539:SER:HB2	1:B:1569:ILE:HG12	2.02	0.42
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	2.01	0.42
1:B:95:VAL:HG22	1:B:115:GLN:HG3	2.02	0.42
1:B:297:ARG:HD3	1:B:320:SER:OG	2.19	0.42
1:A:35:LEU:HG	1:A:35:LEU:O	2.20	0.41
1:A:658:LEU:HD22	1:B:106:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:CD1	1:A:1770:VAL:HG21	2.50	0.41
1:B:323:ARG:CZ	1:B:566:ILE:CG1	2.94	0.41
1:B:1682:ILE:HG22	1:B:1683:ASN:N	2.35	0.41
1:B:1957:SER:OG	1:B:1962:ASP:OD1	2.26	0.41
1:A:297:ARG:NH1	1:A:318:ASP:OD2	2.53	0.41
1:A:334:VAL:HG21	1:A:342:PHE:CE1	2.55	0.41
1:A:990:GLN:HG3	1:A:991:PRO:N	2.35	0.41
1:A:1842:ASP:OD1	1:A:1842:ASP:C	2.62	0.41
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.35	0.41
1:A:73:LYS:HB2	1:A:489:TYR:CE1	2.55	0.41
1:A:1365:MET:O	1:A:1366:SER:C	2.62	0.41
1:A:1703:GLU:OE2	1:A:1703:GLU:N	2.36	0.41
1:A:2086:TYR:HA	1:A:2089:ILE:HD13	2.01	0.41
1:B:1724:THR:O	1:B:1745:ARG:HB2	2.20	0.41
1:A:311:ASN:N	1:A:311:ASN:HD22	2.18	0.41
1:A:2041:LEU:HD13	1:A:2051:TYR:OH	2.19	0.41
1:B:297:ARG:CD	1:B:320:SER:OG	2.67	0.41
1:B:1011:VAL:HG11	1:B:1026:ARG:NH2	2.35	0.41
1:A:799:ALA:HB1	1:A:845:LEU:HD12	2.02	0.41
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.84	0.41
1:A:2093:PHE:O	1:A:2097:HIS:HD2	2.03	0.41
1:B:69:ILE:HG23	1:B:489:TYR:CE1	2.55	0.41
1:B:210:THR:O	1:B:226:ILE:HG21	2.20	0.41
1:B:1044:ILE:HD13	1:B:1075:LEU:HD22	2.01	0.41
1:A:1640:GLN:HB3	1:A:1657:TYR:CZ	2.55	0.41
1:A:1842:ASP:O	1:A:1844:ARG:N	2.54	0.41
1:B:1738:TYR:O	1:B:1742:LEU:HD22	2.20	0.41
1:B:2128:ARG:HG3	1:B:2168:ASP:HA	2.02	0.41
1:A:168:ARG:O	1:A:169:LYS:C	2.63	0.41
1:A:1569:ILE:HG22	1:A:1571:VAL:CG2	2.51	0.41
1:B:323:ARG:NH2	1:B:566:ILE:CG2	2.83	0.41
1:A:819:GLN:O	1:A:820:VAL:C	2.62	0.41
1:A:1603:PHE:O	1:A:1607:VAL:HG23	2.21	0.41
1:A:1683:ASN:C	1:A:1685:GLU:H	2.29	0.41
1:B:147:TRP:CZ2	1:B:149:GLY:HA2	2.55	0.41
1:A:227:TYR:CD1	1:A:227:TYR:C	2.99	0.41
1:A:412:MET:HG3	1:A:418:ILE:HG21	2.03	0.41
1:A:696:VAL:HG12	1:A:696:VAL:O	2.20	0.41
1:A:1624:ASN:ND2	1:A:1732:SER:HA	2.36	0.41
1:A:1629:ILE:HG22	1:B:2024:VAL:HG11	2.03	0.41
1:A:1852:THR:HG22	1:A:1853:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:PHE:O	1:B:806:VAL:HG23	2.20	0.41
1:B:904:VAL:O	1:B:905:GLU:C	2.63	0.41
1:B:933:TYR:OH	1:B:979:ASN:ND2	2.53	0.41
1:B:1471:SER:HB2	1:B:1479:HIS:HD2	1.86	0.41
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.51	0.41
1:A:220:VAL:CG1	1:A:221:SER:N	2.84	0.41
1:A:334:VAL:HG21	1:A:342:PHE:HE1	1.86	0.41
1:A:2037:ARG:O	1:A:2041:LEU:HB2	2.21	0.41
1:A:2159:TYR:OH	1:A:2175:ILE:HD11	2.21	0.41
1:B:196:ALA:HB2	1:B:355:LEU:HD22	2.03	0.41
1:B:485:ASN:CG	1:B:522:HIS:CD2	2.99	0.41
1:B:1052:VAL:HG12	1:B:1053:VAL:N	2.36	0.41
1:B:1232:PHE:CE1	1:B:1241:ARG:HG3	2.55	0.41
1:B:1322:VAL:HG22	1:B:1338:THR:HG23	2.02	0.41
1:A:389:PRO:HA	1:A:392:GLU:HB2	2.03	0.40
1:A:1478:MET:HE2	1:A:1478:MET:HB3	1.92	0.40
1:A:2013:GLU:OE1	1:A:2129:ARG:HD3	2.21	0.40
1:B:202:PRO:HB2	1:B:291:LYS:HB2	2.03	0.40
1:B:684:ARG:HH11	1:B:684:ARG:HB3	1.85	0.40
1:B:835:ASN:HD22	1:B:836:PRO:HD2	1.86	0.40
1:B:2138:ARG:NH2	1:B:2183:ASP:OD2	2.54	0.40
1:A:1597:GLY:O	1:A:1598:PRO:C	2.63	0.40
1:B:1100:ALA:O	1:B:1103:GLN:HB2	2.20	0.40
1:B:1657:TYR:HB3	1:B:1689:VAL:HA	2.02	0.40
1:B:1783:MET:CA	1:B:1786:ASN:HB2	2.45	0.40
1:B:1960:GLN:HE21	1:B:1960:GLN:HB2	1.64	0.40
1:A:625:HIS:O	1:A:626:GLU:HB2	2.21	0.40
1:A:1182:HIS:CE1	1:A:1230:GLU:O	2.71	0.40
1:A:1293:GLU:O	1:A:1294:PRO:C	2.63	0.40
1:B:1239:LEU:O	1:B:1243:ARG:HG2	2.21	0.40
1:A:596:ALA:HB1	1:A:614:LEU:O	2.21	0.40
1:A:955:ARG:NH2	1:A:1914:GLU:OE1	2.46	0.40
1:A:1620:TYR:O	1:A:1726:THR:HA	2.21	0.40
1:A:1940:ASN:ND2	1:A:1981:TYR:HA	2.37	0.40
1:A:2178:ASN:C	1:A:2180:LYS:H	2.29	0.40
1:B:73:LYS:O	1:B:77:SER:OG	2.35	0.40
1:B:1544:GLU:HA	1:B:1549:GLU:O	2.22	0.40
1:A:185:ASP:OD2	1:A:227:TYR:OH	2.27	0.40
1:A:486:VAL:HG11	1:A:526:ALA:HB1	2.01	0.40
1:A:2058:LEU:HD21	1:A:2071:ILE:HB	2.04	0.40
1:B:323:ARG:CZ	1:B:468:PHE:CZ	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:OD1	1:A:440:ASP:OD1[7_466]	1.80	0.40

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	1980/2218 (89%)	1771 (89%)	188 (10%)	21 (1%)	11	39
1	B	1997/2218 (90%)	1778 (89%)	203 (10%)	16 (1%)	16	47
All	All	3977/4436 (90%)	3549 (89%)	391 (10%)	37 (1%)	14	44

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	572	ALA
1	A	184	GLY
1	A	573	GLU
1	A	1316	ASP
1	A	1378	SER
1	A	1591	PHE
1	A	1843	VAL
1	B	184	GLY
1	B	1593	ILE
1	B	1682	ILE
1	A	431	GLU
1	A	1050	SER

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Mol	Chain	Res	Type
1	A	1828	ASP
1	B	1650	ASP
1	B	1744	GLN
1	B	2177	GLU
1	A	1098	THR
1	B	431	GLU
1	B	659	SER
1	B	689	SER
1	B	787	ASP
1	B	851	HIS
1	A	169	LYS
1	A	610	LEU
1	A	689	SER
1	A	898	LYS
1	A	1195	GLU
1	A	1305	LEU
1	A	1731	ARG
1	A	2166	GLU
1	B	1052	VAL
1	B	1769	GLU
1	B	1843	VAL
1	B	2080	ARG
1	A	680	VAL
1	A	783	GLY
1	A	1281	PRO

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	1323/1912 (69%)	1223 (92%)	100 (8%)	12	39
1	B	1735/1912 (91%)	1624 (94%)	111 (6%)	16	44
All	All	3058/3824 (80%)	2847 (93%)	211 (7%)	14	41

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	66	ASN
1	A	567	THR
1	A	602	GLU
1	A	633	THR
1	A	643	THR
1	A	644	LEU
1	A	649	SER
1	A	653	ILE
1	A	659	SER
1	A	670	LYS
1	A	671	SER
1	A	777	HIS
1	A	779	LEU
1	A	790	SER
1	A	793	ILE
1	A	796	THR
1	A	797	LYS
1	A	807	SER
1	A	825	SER
1	A	841	SER
1	A	845	LEU
1	A	852	SER
1	A	883	LYS
1	A	915	SER
1	A	980	ASN
1	A	990	GLN
1	A	1023	LEU
1	A	1044	ILE
1	A	1075	LEU
1	A	1081	VAL
1	A	1180	VAL
1	A	1190	LEU
1	A	1191	SER
1	A	1193	SER
1	A	1223	ASN
1	A	1239	LEU
1	A	1259	ARG
1	A	1282	ASN
1	A	1343	ARG
1	A	1350	ASP
1	A	1364	LEU
1	A	1390	ILE

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Mol	Chain	Res	Type
1	A	1413	LYS
1	A	1417	ARG
1	A	1419	ARG
1	A	1433	GLN
1	A	1434	THR
1	A	1489	VAL
1	A	1516	ARG
1	A	1546	GLU
1	A	1562	ILE
1	A	1565	VAL
1	A	1571	VAL
1	A	1583	VAL
1	A	1585	VAL
1	A	1589	ILE
1	A	1592	LYS
1	A	1602	GLU
1	A	1616	ILE
1	A	1660	SER
1	A	1686	GLU
1	A	1691	LYS
1	A	1726	THR
1	A	1732	SER
1	A	1735	ILE
1	A	1755	ILE
1	A	1764	LYS
1	A	1777	LEU
1	A	1781	GLN
1	A	1791	LEU
1	A	1792	THR
1	A	1797	LEU
1	A	1824	LYS
1	A	1843	VAL
1	A	1854	SER
1	A	1884	LEU
1	A	1912	SER
1	A	1924	TRP
1	A	1968	LEU
1	A	1991	PRO
1	A	2001	VAL
1	A	2018	VAL
1	A	2021	ARG
1	A	2025	LEU

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Mol	Chain	Res	Type
1	A	2027	PRO
1	A	2041	LEU
1	A	2043	THR
1	A	2053	GLU
1	A	2083	LEU
1	A	2089	ILE
1	A	2090	SER
1	A	2114	GLU
1	A	2117	GLU
1	A	2119	ARG
1	A	2127	ARG
1	A	2149	LEU
1	A	2180	LYS
1	A	2186	LEU
1	A	2187	LYS
1	B	37	THR
1	B	66	ASN
1	B	108	GLU
1	B	124	ASN
1	B	195	SER
1	B	269	GLU
1	B	319	CYS
1	B	335	THR
1	B	360	SER
1	B	367	LEU
1	B	457	CYS
1	B	471	SER
1	B	508	HIS
1	B	531	SER
1	B	545	LYS
1	B	557	ILE
1	B	605	GLN
1	B	633	THR
1	B	643	THR
1	B	653	ILE
1	B	673	THR
1	B	684	ARG
1	B	782	GLU
1	B	784	MET
1	B	785	LEU
1	B	801	LYS
1	B	845	LEU

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Mol	Chain	Res	Type
1	B	848	SER
1	B	853	ARG
1	B	883	LYS
1	B	886	ASP
1	B	924	SER
1	B	967	LEU
1	B	975	VAL
1	B	990	GLN
1	B	997	SER
1	B	1015	SER
1	B	1040	ARG
1	B	1057	TYR
1	B	1084	ASP
1	B	1108	ARG
1	B	1176	ILE
1	B	1180	VAL
1	B	1190	LEU
1	B	1191	SER
1	B	1223	ASN
1	B	1343	ARG
1	B	1344	THR
1	B	1350	ASP
1	B	1359	SER
1	B	1364	LEU
1	B	1380	SER
1	B	1390	ILE
1	B	1409	GLU
1	B	1430	LYS
1	B	1434	THR
1	B	1437	PRO
1	B	1466	GLU
1	B	1477	SER
1	B	1499	LYS
1	B	1506	THR
1	B	1508	VAL
1	B	1521	SER
1	B	1533	THR
1	B	1534	ASP
1	B	1539	SER
1	B	1542	LEU
1	B	1550	LEU
1	B	1565	VAL

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Mol	Chain	Res	Type
1	B	1568	LYS
1	B	1571	VAL
1	B	1580	ARG
1	B	1583	VAL
1	B	1585	VAL
1	B	1616	ILE
1	B	1634	GLU
1	B	1651	LYS
1	B	1653	PHE
1	B	1664	GLU
1	B	1665	THR
1	B	1667	LYS
1	B	1680	THR
1	B	1681	VAL
1	B	1683	ASN
1	B	1705	LEU
1	B	1731	ARG
1	B	1735	ILE
1	B	1740	VAL
1	B	1741	ARG
1	B	1742	LEU
1	B	1764	LYS
1	B	1777	LEU
1	B	1781	GLN
1	B	1786	ASN
1	B	1792	THR
1	B	1802	LYS
1	B	1808	SER
1	B	1843	VAL
1	B	1875	LYS
1	B	1915	THR
1	B	1920	PRO
1	B	1945	LEU
1	B	1960	GLN
1	B	1980	ASP
1	B	1992	THR
1	B	2031	VAL
1	B	2037	ARG
1	B	2101	SER
1	B	2106	LYS
1	B	2162	SER
1	B	2192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	66	ASN
1	A	828	GLN
1	A	880	GLN
1	A	979	ASN
1	A	980	ASN
1	A	988	HIS
1	A	1031	GLN
1	A	1043	GLN
1	A	1182	HIS
1	A	1321	HIS
1	A	1354	GLN
1	A	1384	HIS
1	A	1433	GLN
1	A	1605	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1648	ASN
1	A	1654	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1781	GLN
1	A	1934	GLN
1	A	1941	ASN
1	A	1944	GLN
1	A	2011	GLN
1	A	2060	ASN
1	A	2074	GLN
1	A	2092	GLN
1	A	2097	HIS
1	B	31	HIS
1	B	36	ASN
1	B	53	HIS
1	B	66	ASN
1	B	124	ASN
1	B	152	HIS
1	B	228	GLN
1	B	280	ASN
1	B	298	HIS
1	B	370	HIS
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	445	GLN
1	B	453	HIS
1	B	499	HIS
1	B	508	HIS
1	B	522	HIS
1	B	608	GLN
1	B	616	GLN
1	B	835	ASN
1	B	941	ASN
1	B	979	ASN
1	B	988	HIS
1	B	1070	ASN
1	B	1088	GLN
1	B	1092	HIS
1	B	1249	ASN
1	B	1279	ASN
1	B	1384	HIS
1	B	1479	HIS
1	B	1522	GLN
1	B	1605	ASN
1	B	1648	ASN
1	B	1683	ASN
1	B	1748	GLN
1	B	1774	ASN
1	B	1781	GLN
1	B	1786	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1925	HIS
1	B	1934	GLN
1	B	1941	ASN
1	B	1960	GLN
1	B	1983	GLN
1	B	2045	ASN
1	B	2057	GLN
1	B	2074	GLN
1	B	2088	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](#)

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1996/2218 (89%)	-0.06	32 (1%)	70 49	47, 85, 140, 237	0
1	B	2017/2218 (90%)	-0.02	34 (1%)	69 48	46, 87, 161, 237	0
All	All	4013/4436 (90%)	-0.04	66 (1%)	70 49	46, 86, 150, 237	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	945	VAL	5.5
1	B	1197	ILE	3.9
1	A	856	ALA	3.7
1	B	2182	LEU	3.4
1	B	794	GLU	3.3
1	B	1136	PRO	3.2
1	B	272	ILE	3.2
1	B	323	ARG	3.1
1	B	1137	SER	3.0
1	B	897	ASP	3.0
1	B	262	ILE	2.9
1	B	2181	THR	2.9
1	B	293	ALA	2.9
1	A	793	ILE	2.9
1	A	899	LEU	2.8
1	A	1680	THR	2.8
1	B	1162	SER	2.7
1	A	870	LEU	2.7
1	B	330	GLU	2.7
1	A	897	ASP	2.6
1	B	899	LEU	2.6
1	A	894	TYR	2.6
1	B	28	LEU	2.6
1	B	226	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	870	LEU	2.6
1	A	2146	ALA	2.6
1	A	2181	THR	2.6
1	A	670	LYS	2.6
1	A	689	SER	2.5
1	A	797	LYS	2.5
1	B	2191	LEU	2.5
1	A	2186	LEU	2.5
1	B	1127	PRO	2.5
1	B	1058	GLY	2.5
1	A	517	GLN	2.4
1	B	449	ILE	2.4
1	B	200	CYS	2.4
1	A	1648	ASN	2.4
1	A	282	ILE	2.4
1	B	696	VAL	2.4
1	A	225	ASP	2.3
1	A	2152	ILE	2.3
1	B	2179	TYR	2.3
1	A	1171	PRO	2.3
1	A	779	LEU	2.3
1	A	2187	LYS	2.3
1	B	1187	ASP	2.3
1	B	189	SER	2.2
1	A	854	LEU	2.2
1	A	900	LEU	2.2
1	B	874	ALA	2.2
1	A	1430	LYS	2.2
1	A	2182	LEU	2.2
1	B	29	PRO	2.2
1	A	1127	PRO	2.1
1	A	795	GLY	2.1
1	A	1409	GLU	2.1
1	A	1602	GLU	2.1
1	B	340	GLU	2.1
1	B	1057	TYR	2.1
1	A	1681	VAL	2.1
1	B	1255	ASN	2.1
1	B	370	HIS	2.0
1	A	1196	VAL	2.0
1	A	514	GLU	2.0
1	B	367	LEU	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.