



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:59 PM UTC

PDB ID : 1SDD / pdb_00001sdd
Title : Crystal Structure of Bovine Factor Vai
Authors : Adams, T.E.; Hockin, M.F.; Mann, K.G.; Everse, S.J.
Deposited on : 2004-02-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

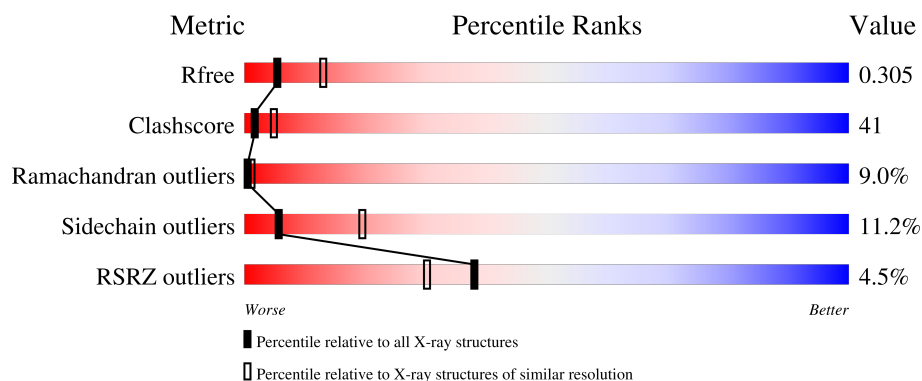
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	306	
2	B	647	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2187	X	-	-	-
3	NAG	B	2189	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7271 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.

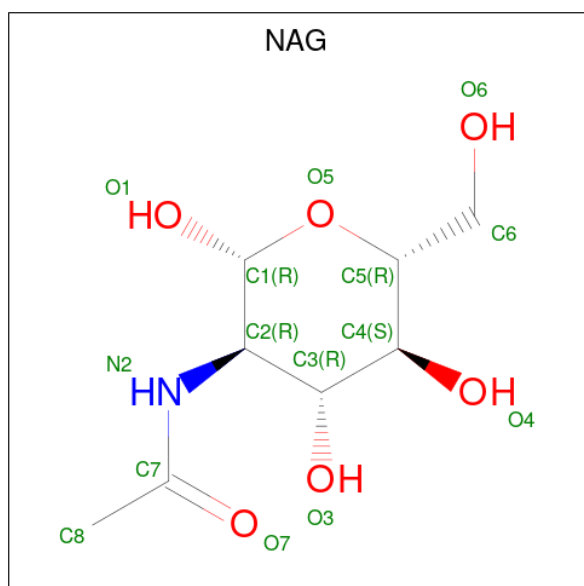
- Molecule 1 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2132	1366	356	398	12			

- Molecule 2 is a protein called Coagulation factor V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	601	Total	C	N	O	S	0	0	0
			4878	3127	840	888	23			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cu	0	0
			1	1		

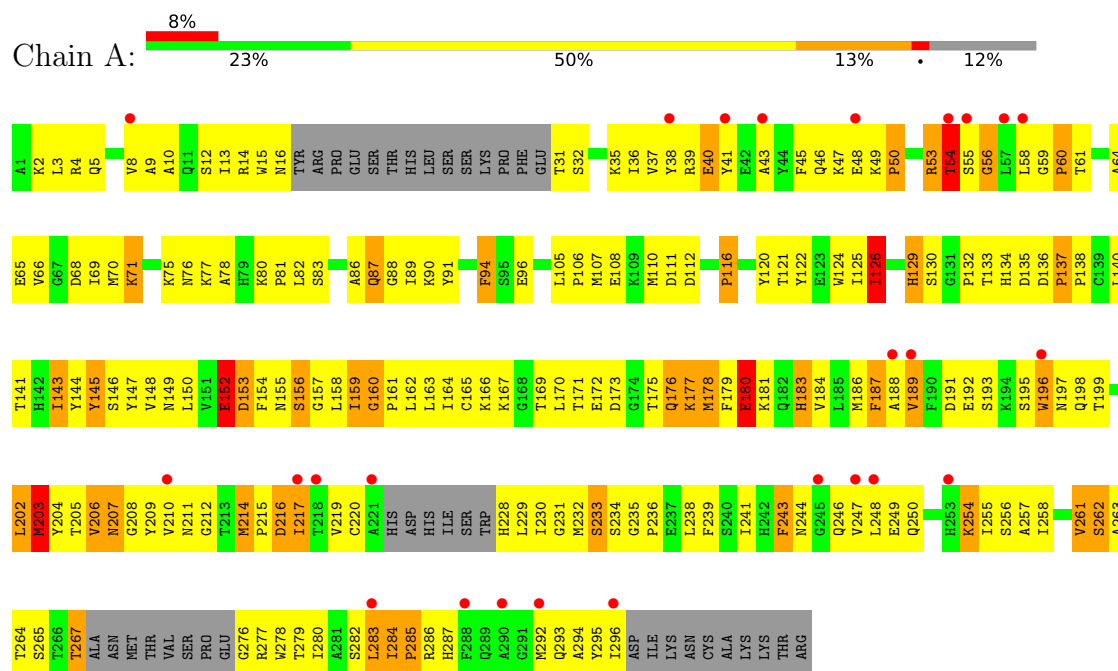
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	142	Total	O	0	0
			142	142		

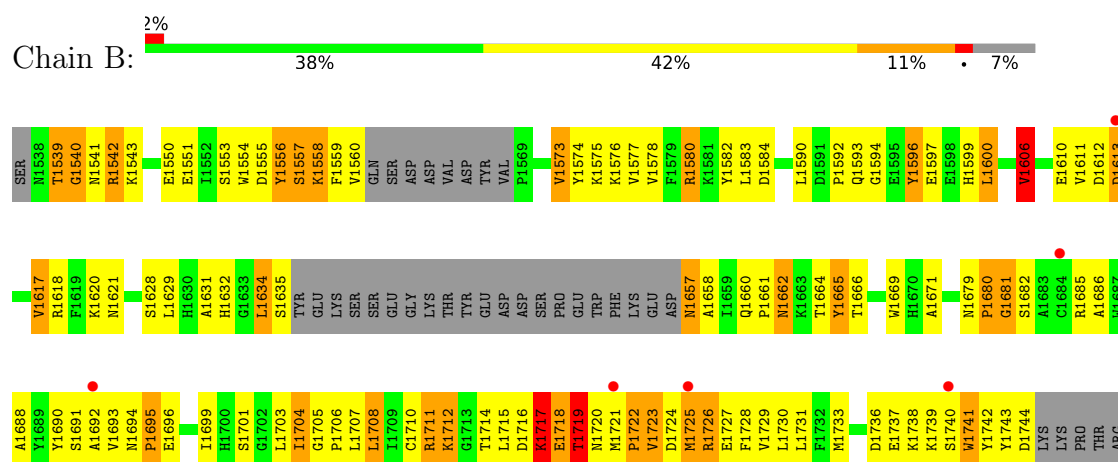
3 Residue-property plots

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

• Molecule 1: Coagulation factor V



• Molecule 2: Coagulation factor V



V2147	K2148	F2151	N2152	P2153	P2154	I2155	I2160	R2161	I2162	T2166	W2167	N2168	Q2169	S2170	I2171	A2172	R2173	R2174	L2175		F2178	G2179	C2180	D2181	M2182	TYR	SER	TRP	ARG	ARG	ALA	SER	SER	GLU	VAL	LYS	N1760		H1765	A1766	I1767	M1770	I1771	Y1772	N1773	L1774		Y1780	E1781	Q1782	E1783	W1784	V1785	R1786	L1787	H1788	L1789	L1790	N1791	L1792	G1793	G1794	D1797	I1798		V1801	H1802	F1803	H1804	G1805	Q1806	T1807	L1808	L1809	E1810	N1811	G1812	T1813	Q1814	Q1815	H1816	Q1817	L1818	G1819
V1820	W1821	P1822	L1823		L1831	E1832	M1833	K1834	A1835	S1836	X1837	L1843	D1844	T1845	E1846	V1847	G1848	E1849	I1850	Q1851	R1852	A1853	G1854	W1855	Q1856	T1857	L1860	I1861		R1864	K1867	M1868	P1869	M1870	G1871	L1872		L1876	I1877		E1886	F1887	W1888	G1889	Y1890	W1891	E1892	P1893	K1894	L1895	A1896	R1897	L1898	N1899	N1900																													
Y1904	M1905	A1906		K1911	L1912	S1913	T1914	F1916	E1915	N1917	P1918	E1919	P1920	W1921	D1925	M1926	Q1927	K1928		L1931		I1935		Q1938	G1939		H1942	Y1943	L1944	K1945	P1946		T1950	E1951		D1959	R1960		W1963	R1964	I1965	F1966	K1967	G1968	N1969	S1970		N1973	V1974		E1988		I1991	D1992	P1993		R1998	Y1999																										
I2000	R2001	I2002	S2003	P2004		Y2008	M2009	K2010	P2011	A2012	L2013	R2014	L2015	E2016	L2017	Q2018	G2019	V2022	C2025	S2026	T2027	G2030	M2031		G2034	K2035	I2036	E2037	N2038	K2039	Q2040	I2041		S2044	S2045	F2046	K2047	K2048	S2049	W2050	W2051	G2052	N2053	Y2054	W2055	E2056	P2057	F2058	L2059		L2062	N2063	R2067	N2069																														
A2070	W2071	Q2072	K2073	A2075	N2077	N2078		W2081	L2082	Q2083	T2084	D2085	L2086	L2087	K2088	L2089	K2090	K2091	L2092	T2093		V2096	T2097	Q2098	G2099	K2100	C2101	E2106	P2107	Y2108	V2109	K2110	S2111	Y2112	T2113		D2118		T2121	D2122	W2123	P2124	F2125	Y2126	R2127	E2128		N2132		N2140	N2141	N2142	Y2143	R2144	G2145	H2146																												

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.37Å 86.56Å 229.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-2.80) 90.5 (30.00-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.296 0.248 , 0.305	Depositor DCC
R_{free} test set	918 reflections (3.19%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7271	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CA, NAG

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	0.40	0/2188	0.91	8/2960 (0.3%)
2	B	0.55	0/5012	1.02	31/6792 (0.5%)
All	All	0.51	0/7200	0.99	39/9752 (0.4%)

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
2	B	0	1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2014	ARG	N-CA-C	-9.03	93.53	108.34
2	B	1556	TYR	N-CA-C	-8.98	98.75	110.33
2	B	2143	VAL	N-CA-C	8.96	119.77	110.72
2	B	1837	LYS	CA-C-N	8.31	128.81	119.92
2	B	1837	LYS	C-N-CA	8.31	128.81	119.92
2	B	1847	VAL	N-CA-C	-8.21	93.11	106.32
2	B	1741	TRP	N-CA-C	-8.04	101.65	112.26
2	B	1766	ALA	N-CA-C	6.95	120.44	109.81
2	B	1857	THR	CA-C-N	-6.38	114.06	120.31
2	B	1857	THR	C-N-CA	-6.38	114.06	120.31
2	B	1813	THR	N-CA-C	-6.25	105.75	113.19
2	B	2056	GLU	CA-C-N	6.08	125.80	119.05
2	B	2056	GLU	C-N-CA	6.08	125.80	119.05
2	B	2173	LEU	N-CA-C	6.01	118.21	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2153	PRO	N-CA-C	-5.99	103.39	110.70
1	A	160	GLY	CA-C-N	5.99	125.93	119.76
1	A	160	GLY	C-N-CA	5.99	125.93	119.76
2	B	1998	ARG	N-CA-C	-5.94	106.64	114.31
2	B	1681	GLY	N-CA-C	5.87	122.86	112.64
2	B	1584	ASP	N-CA-C	5.81	115.91	108.24
2	B	1606	VAL	N-CA-C	5.79	115.59	107.37
2	B	1860	LEU	N-CA-C	5.52	118.24	109.24
2	B	1719	THR	N-CA-C	5.50	122.52	110.80
2	B	1553	SER	N-CA-C	-5.47	100.79	109.76
1	A	54	THR	CB-CA-C	-5.42	108.75	116.34
2	B	1767	ILE	N-CA-C	-5.34	100.42	108.12
1	A	202	LEU	N-CA-C	-5.31	103.88	110.41
1	A	121	THR	N-CA-C	5.27	117.31	107.99
2	B	2015	LEU	N-CA-C	5.26	116.98	109.14
2	B	2012	ALA	N-CA-C	-5.24	102.30	110.42
2	B	2152	ASN	CA-C-N	-5.24	114.99	120.38
2	B	2152	ASN	C-N-CA	-5.24	114.99	120.38
1	A	284	ILE	CA-C-N	5.17	126.31	119.84
1	A	284	ILE	C-N-CA	5.17	126.31	119.84
2	B	1892	GLU	CA-C-N	5.13	125.17	119.32
2	B	1892	GLU	C-N-CA	5.13	125.17	119.32
2	B	2145	GLY	N-CA-C	5.10	117.79	111.93
2	B	2035	LYS	N-CA-C	-5.09	105.17	111.33
1	A	40	GLU	N-CA-C	5.03	119.61	111.37

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1890	TYR	Sidechain

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	2132	0	2074	213	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4878	0	4767	372	0
3	A	28	0	26	3	0
3	B	42	0	39	11	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	47	0	0	1	0
6	B	142	0	0	3	0
All	All	7271	0	6906	578	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 41.

All (578) 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)
2:B:1992:ASP:HB3	2:B:1993:PRO:HD3	1.13	1.13
2:B:2152:ASN:HB2	2:B:2153:PRO:HD3	1.22	1.10
2:B:1721:MET:HG3	2:B:1786:ARG:HH22	1.01	1.08
2:B:1914:THR:HB	2:B:1920:PRO:HD2	1.38	1.05
1:A:264:THR:HG21	2:B:1822:PRO:HG3	1.44	0.98
2:B:1597:GLU:HB2	2:B:1600:LEU:HD22	1.46	0.97
2:B:1542:ARG:H	2:B:1542:ARG:CZ	1.78	0.96
2:B:1992:ASP:CB	2:B:1993:PRO:HD3	1.93	0.95
2:B:1721:MET:HG3	2:B:1786:ARG:NH2	1.81	0.94
1:A:229:LEU:HD23	1:A:241:ILE:HD12	1.51	0.92
2:B:1542:ARG:H	2:B:1542:ARG:NE	1.69	0.91
2:B:1580:ARG:HG2	2:B:1580:ARG:HH11	1.30	0.91
2:B:2067:ARG:HA	2:B:2067:ARG:HH11	1.33	0.90
2:B:1893:PRO:HD2	2:B:1894:LYS:HZ1	1.37	0.87
2:B:1721:MET:HE3	2:B:1786:ARG:HH12	1.37	0.86
1:A:94:PHE:HE2	2:B:2182:MET:HE2	1.39	0.85
2:B:1894:LYS:H	2:B:1894:LYS:HE2	1.40	0.85
2:B:1628:SER:O	2:B:1691:SER:HA	1.77	0.84
2:B:2152:ASN:HB2	2:B:2153:PRO:CD	2.08	0.83
2:B:1868:MET:HE1	2:B:2027:THR:HA	1.58	0.83
2:B:1893:PRO:HD2	2:B:1894:LYS:NZ	1.92	0.83
1:A:198:GLN:HB2	3:A:2185:NAG:H81	1.59	0.82
1:A:140:LEU:HA	1:A:267:THR:HG21	1.62	0.82
2:B:2030:GLY:HA3	2:B:2036:ILE:HG13	1.61	0.82
2:B:1721:MET:HE1	2:B:1723:VAL:HB	1.61	0.81
1:A:4:ARG:HH22	1:A:170:LEU:HD23	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2168:ASN:C	2:B:2168:ASN:HD22	1.90	0.80
1:A:91:TYR:CE1	1:A:96:GLU:HG3	2.17	0.80
2:B:1721:MET:CG	2:B:1786:ARG:HH22	1.91	0.80
2:B:1911:LYS:HD2	2:B:1911:LYS:O	1.83	0.79
2:B:2096:VAL:HG23	2:B:2178:PHE:HE1	1.48	0.79
2:B:1992:ASP:HB3	2:B:1993:PRO:CD	2.07	0.79
2:B:2111:SER:HB2	2:B:2166:THR:HG22	1.63	0.78
1:A:214:MET:HE1	1:A:295:TYR:CE2	2.19	0.78
2:B:2162:ILE:HD12	2:B:2162:ILE:N	1.99	0.78
2:B:1905:ASN:H	2:B:1905:ASN:HD22	1.32	0.77
2:B:2083:GLN:HB3	2:B:2161:ARG:HG2	1.67	0.76
1:A:197:ASN:HD21	3:A:2185:NAG:H4	1.50	0.76
2:B:1808:LEU:HB3	2:B:1831:LEU:HD12	1.68	0.76
1:A:232:MET:HA	1:A:262:SER:O	1.87	0.75
2:B:2096:VAL:HG23	2:B:2178:PHE:CE1	2.21	0.75
2:B:1917:ASN:HD21	2:B:1919:GLU:HB2	1.52	0.75
1:A:167:LYS:H	1:A:167:LYS:HD2	1.51	0.75
2:B:1915:GLU:C	2:B:1917:ASN:H	1.95	0.74
1:A:279:THR:HA	1:A:295:TYR:HA	1.69	0.73
2:B:1593:GLN:HG3	2:B:1597:GLU:HG3	1.70	0.73
2:B:2152:ASN:CB	2:B:2153:PRO:HD3	2.11	0.73
1:A:161:PRO:HG2	1:A:184:VAL:HG11	1.69	0.73
2:B:1680:PRO:HG2	2:B:1813:THR:HA	1.70	0.73
2:B:1580:ARG:HG2	2:B:1580:ARG:NH1	1.95	0.73
2:B:2071:TRP:O	2:B:2172:ALA:HA	1.88	0.73
2:B:1692:ALA:O	2:B:1695:PRO:HD3	1.89	0.72
1:A:141:THR:OG1	1:A:267:THR:HB	1.89	0.72
2:B:1685:ARG:HD2	2:B:1686:ALA:H	1.55	0.71
1:A:133:THR:HG22	1:A:134:HIS:H	1.55	0.71
2:B:2126:TYR:OH	2:B:2153:PRO:HD2	1.91	0.71
1:A:90:LYS:HZ1	2:B:1807:THR:HB	1.55	0.71
1:A:162:LEU:O	1:A:163:LEU:HD23	1.91	0.70
2:B:1706:PRO:HB3	2:B:1729:VAL:HG11	1.73	0.70
1:A:202:LEU:HD23	1:A:203:MET:H	1.57	0.70
2:B:2101:LYS:HD3	2:B:2144:ARG:NH2	2.07	0.69
2:B:1742:TYR:C	2:B:1744:ASP:H	1.98	0.69
2:B:2055:TRP:HB2	2:B:2072:GLN:HB2	1.73	0.69
1:A:159:ILE:HD13	1:A:186:MET:SD	2.32	0.68
1:A:80:LYS:NZ	1:A:152:GLU:HG2	2.08	0.68
1:A:146:SER:HB3	1:A:153:ASP:OD1	1.93	0.68
1:A:264:THR:CG2	2:B:1822:PRO:HG3	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1927:GLN:C	2:B:1998:ARG:HE	2.01	0.68
2:B:1577:VAL:HG22	2:B:1703:LEU:HD21	1.75	0.67
2:B:1680:PRO:O	3:B:2188:NAG:H62	1.94	0.67
2:B:1725:MET:HG2	2:B:1726:ARG:N	2.10	0.67
1:A:37:VAL:HG11	1:A:39:ARG:NH1	2.10	0.66
2:B:2168:ASN:HD22	2:B:2169:GLN:N	1.93	0.66
2:B:1727:GLU:CD	2:B:1786:ARG:HH21	2.04	0.66
2:B:1541:ASN:HA	2:B:1542:ARG:HH21	1.61	0.65
2:B:2101:LYS:NZ	2:B:2144:ARG:HH22	1.94	0.65
1:A:37:VAL:HG11	1:A:39:ARG:HH11	1.60	0.65
2:B:2110:LYS:HB2	2:B:2166:THR:HG23	1.78	0.65
2:B:1542:ARG:NE	2:B:1542:ARG:N	2.44	0.65
1:A:177:LYS:HE3	1:A:178:MET:HE3	1.78	0.65
2:B:2111:SER:CB	2:B:2166:THR:HG22	2.26	0.65
1:A:71:LYS:HB2	1:A:71:LYS:NZ	2.12	0.65
2:B:1998:ARG:HD3	2:B:1999:TYR:CE1	2.32	0.65
1:A:206:VAL:O	1:A:207:ASN:HB2	1.96	0.65
2:B:1543:LYS:HD2	6:B:2358:HOH:O	1.97	0.65
2:B:2092:ILE:HG22	2:B:2151:PHE:HE2	1.62	0.64
2:B:1724:ASP:O	2:B:1725:MET:O	2.15	0.64
2:B:1664:THR:HG22	2:B:1665:TYR:H	1.63	0.64
2:B:1821:TRP:HZ3	2:B:1823:LEU:HD23	1.62	0.63
2:B:2002:ILE:HD12	2:B:2015:LEU:HD22	1.80	0.63
2:B:1890:TYR:HB3	2:B:1904:TYR:CE2	2.34	0.63
2:B:1721:MET:CE	2:B:1723:VAL:HB	2.28	0.63
2:B:1803:PHE:CD2	2:B:1808:LEU:HD11	2.34	0.63
2:B:1969:ASN:OD1	3:B:2189:NAG:N2	2.30	0.63
1:A:132:PRO:HA	1:A:140:LEU:HD11	1.79	0.63
1:A:255:ILE:HD11	1:A:258:ILE:HG12	1.79	0.63
2:B:1541:ASN:OD1	2:B:1542:ARG:NH2	2.31	0.63
2:B:1931:LEU:HD12	2:B:2022:VAL:HA	1.80	0.63
2:B:1988:GLU:H	2:B:1988:GLU:CD	2.07	0.62
2:B:2091:LYS:O	2:B:2179:GLY:HA3	1.99	0.62
1:A:4:ARG:NH2	1:A:170:LEU:HD23	2.13	0.62
1:A:38:TYR:O	1:A:39:ARG:HD2	2.00	0.62
2:B:2090:LYS:HE2	2:B:2181:ASP:OD2	1.98	0.62
2:B:1963:TRP:CZ3	2:B:2001:ARG:HB2	2.34	0.62
2:B:1894:LYS:H	2:B:1894:LYS:CE	2.11	0.62
2:B:1898:LEU:HD22	2:B:1938:GLN:OE1	1.99	0.62
1:A:71:LYS:HB2	1:A:71:LYS:HZ2	1.65	0.62
1:A:76:ASN:ND2	1:A:116:PRO:HA	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PRO:HG3	1:A:230:ILE:CD1	2.30	0.61
1:A:231:GLY:O	1:A:239:PHE:HE2	1.84	0.61
2:B:1662:ASN:HB2	3:B:2187:NAG:H5	1.81	0.61
1:A:48:GLU:HG3	1:A:50:PRO:HD3	1.82	0.61
2:B:1765:HIS:HD2	2:B:1850:ILE:HG23	1.66	0.61
2:B:2076:ASN:OD1	2:B:2170:SER:HA	2.00	0.61
2:B:2110:LYS:HD3	2:B:2167:TRP:O	2.00	0.61
1:A:107:MET:HA	1:A:110:MET:HE2	1.81	0.61
2:B:1610:GLU:O	2:B:1613:ASP:HB2	2.01	0.61
2:B:2049:SER:HB2	2:B:2051:TRP:CE3	2.35	0.61
2:B:1543:LYS:HD2	2:B:1719:THR:HG21	1.83	0.60
1:A:94:PHE:CE2	2:B:2182:MET:HE2	2.30	0.60
2:B:1725:MET:HG2	2:B:1726:ARG:H	1.65	0.60
2:B:1911:LYS:HD2	2:B:1911:LYS:C	2.26	0.60
1:A:186:MET:HE3	1:A:188:ALA:HB3	1.83	0.60
1:A:203:MET:O	1:A:205:THR:HG23	2.01	0.60
2:B:1803:PHE:CE1	2:B:1843:LEU:HD13	2.35	0.60
2:B:2109:VAL:HG21	2:B:2173:LEU:HG	1.83	0.60
2:B:1629:LEU:HD22	2:B:1669:TRP:HH2	1.64	0.60
2:B:2110:LYS:HD3	2:B:2167:TRP:C	2.26	0.60
2:B:1657:ASN:C	2:B:1657:ASN:HD22	2.10	0.60
2:B:1681:GLY:HA2	3:B:2188:NAG:H62	1.81	0.60
2:B:1662:ASN:HB2	3:B:2187:NAG:C5	2.32	0.60
2:B:1844:ASP:HB2	2:B:1851:GLN:HG3	1.84	0.60
2:B:1780:TYR:O	2:B:1783:GLU:HB3	2.03	0.59
1:A:87:GLN:HG3	1:A:87:GLN:O	2.03	0.59
2:B:1685:ARG:HD2	2:B:1686:ALA:N	2.17	0.59
2:B:2008:TYR:O	2:B:2009:ASN:HB2	2.01	0.59
2:B:2092:ILE:HB	2:B:2155:ILE:HB	1.84	0.59
1:A:90:LYS:NZ	2:B:1807:THR:HB	2.17	0.59
1:A:278:TRP:O	1:A:296:ILE:N	2.34	0.59
2:B:2037:GLU:O	2:B:2040:GLN:HB2	2.03	0.59
1:A:80:LYS:HZ1	1:A:152:GLU:HG2	1.66	0.59
2:B:1631:ALA:HB2	2:B:1669:TRP:CH2	2.38	0.59
1:A:236:PRO:HG3	2:B:1850:ILE:HD11	1.83	0.59
1:A:38:TYR:C	1:A:39:ARG:HD2	2.28	0.59
1:A:206:VAL:HG11	1:A:294:ALA:HB2	1.83	0.59
2:B:1731:LEU:HD12	2:B:1790:LEU:O	2.03	0.59
2:B:2055:TRP:CB	2:B:2072:GLN:HB2	2.31	0.58
2:B:1551:GLU:OE2	2:B:1741:TRP:CH2	2.56	0.58
2:B:1620:LYS:O	2:B:1621:ASN:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1680:PRO:HG2	2:B:1813:THR:CA	2.33	0.58
2:B:1912:LEU:HD23	2:B:2011:PRO:HG3	1.86	0.58
1:A:206:VAL:O	1:A:206:VAL:HG12	2.03	0.58
1:A:14:ARG:HG3	1:A:32:SER:HB3	1.86	0.58
2:B:2167:TRP:CZ3	2:B:2171:ILE:HD11	2.39	0.58
1:A:167:LYS:HD2	1:A:167:LYS:N	2.19	0.57
2:B:1765:HIS:CD2	2:B:1850:ILE:HG23	2.39	0.57
2:B:1634:LEU:HD23	2:B:1635:SER:N	2.19	0.57
2:B:2038:ASN:C	2:B:2040:GLN:H	2.12	0.57
2:B:1803:PHE:HD2	2:B:1808:LEU:HD11	1.69	0.57
1:A:197:ASN:HD21	3:A:2185:NAG:C4	2.16	0.57
2:B:1942:HIS:HD1	2:B:1943:TYR:HD1	1.51	0.57
1:A:158:LEU:O	1:A:159:ILE:HB	2.03	0.57
1:A:186:MET:HG2	1:A:186:MET:O	2.03	0.57
1:A:229:LEU:N	1:A:229:LEU:HD12	2.20	0.57
2:B:1742:TYR:C	2:B:1744:ASP:N	2.63	0.56
2:B:1887:PHE:CD1	2:B:1887:PHE:N	2.73	0.56
1:A:143:ILE:CG2	1:A:265:SER:HB3	2.35	0.56
2:B:2081:TRP:CZ3	2:B:2083:GLN:HG2	2.39	0.56
1:A:132:PRO:HG3	1:A:140:LEU:HG	1.87	0.56
1:A:177:LYS:C	1:A:179:PHE:H	2.13	0.56
2:B:1596:TYR:HD2	2:B:1596:TYR:N	2.04	0.56
1:A:186:MET:O	1:A:188:ALA:N	2.38	0.56
1:A:155:ASN:C	1:A:157:GLY:H	2.12	0.56
2:B:1959:ASP:O	2:B:1960:ARG:CB	2.54	0.56
2:B:1921:TRP:C	2:B:1921:TRP:CD1	2.84	0.56
1:A:145:TYR:N	1:A:145:TYR:CD1	2.73	0.56
2:B:1629:LEU:HD22	2:B:1669:TRP:CH2	2.39	0.56
2:B:1912:LEU:C	2:B:1914:THR:H	2.13	0.56
1:A:60:PRO:HD2	1:A:144:TYR:OH	2.05	0.56
1:A:75:LYS:HE3	1:A:77:LYS:HE3	1.86	0.56
1:A:133:THR:HG22	1:A:134:HIS:N	2.21	0.56
1:A:171:THR:HG22	1:A:173:ASP:H	1.70	0.56
1:A:212:GLY:HA2	1:A:214:MET:SD	2.46	0.56
2:B:1704:ILE:CD1	2:B:1792:LEU:HD12	2.36	0.56
2:B:2101:LYS:HZ3	2:B:2144:ARG:HH22	1.53	0.56
1:A:9:ALA:HB1	1:A:75:LYS:O	2.06	0.55
2:B:1912:LEU:O	2:B:1914:THR:N	2.38	0.55
2:B:1992:ASP:CB	2:B:1993:PRO:CD	2.75	0.55
1:A:284:ILE:O	1:A:286:ARG:N	2.39	0.55
2:B:1596:TYR:N	2:B:1596:TYR:CD2	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1892:GLU:O	2:B:1895:LEU:HB2	2.06	0.55
2:B:2075:ALA:C	2:B:2076:ASN:HD22	2.14	0.55
1:A:238:LEU:H	1:A:238:LEU:HD23	1.71	0.55
1:A:248:LEU:HD11	1:A:256:SER:O	2.06	0.55
2:B:1596:TYR:CE2	2:B:1597:GLU:HG2	2.41	0.55
1:A:86:ALA:HB2	1:A:124:TRP:CH2	2.41	0.55
2:B:1694:ASN:C	2:B:1694:ASN:HD22	2.14	0.55
1:A:189:VAL:HB	1:A:204:TYR:HD1	1.72	0.55
2:B:1543:LYS:HE2	2:B:1543:LYS:HA	1.87	0.55
2:B:1543:LYS:CD	2:B:1719:THR:HG21	2.37	0.55
2:B:1721:MET:HE1	2:B:1724:ASP:H	1.71	0.55
2:B:1812:GLY:C	2:B:1814:GLN:H	2.13	0.55
1:A:66:VAL:HG21	1:A:167:LYS:HE3	1.89	0.55
1:A:138:PRO:HG2	1:A:179:PHE:CE2	2.41	0.55
1:A:249:GLU:OE2	1:A:254:LYS:HB3	2.07	0.55
2:B:2086:LEU:C	2:B:2088:LYS:H	2.14	0.55
1:A:250:GLN:OE1	1:A:255:ILE:HD13	2.06	0.55
2:B:2025:CYS:SG	2:B:2091:LYS:HD3	2.47	0.55
2:B:2048:LYS:HG2	2:B:2054:TYR:HD2	1.70	0.55
2:B:2112:TYR:CD2	2:B:2112:TYR:N	2.74	0.55
1:A:3:LEU:C	1:A:3:LEU:HD23	2.32	0.54
1:A:91:TYR:CZ	1:A:96:GLU:HG3	2.40	0.54
1:A:261:VAL:O	1:A:263:ALA:N	2.41	0.54
1:A:278:TRP:HB2	1:A:296:ILE:HD12	1.89	0.54
2:B:1681:GLY:HA3	2:B:1811:ASN:OD1	2.08	0.54
2:B:1704:ILE:HD13	2:B:1731:LEU:HD22	1.88	0.54
1:A:254:LYS:HD3	1:A:254:LYS:C	2.32	0.54
2:B:1782:GLN:NE2	2:B:1834:LYS:HE2	2.23	0.54
2:B:2039:LYS:HZ3	2:B:2039:LYS:H	1.55	0.54
2:B:1906:ALA:HB2	2:B:2014:ARG:HG3	1.89	0.54
2:B:1915:GLU:C	2:B:1917:ASN:N	2.65	0.54
2:B:2071:TRP:HE3	2:B:2173:LEU:HB2	1.72	0.54
2:B:1606:VAL:HG22	2:B:1606:VAL:O	2.08	0.54
1:A:149:ASN:C	1:A:149:ASN:HD22	2.16	0.54
2:B:1596:TYR:HD2	2:B:1596:TYR:H	1.55	0.54
2:B:1817:GLN:HE21	2:B:1817:GLN:HA	1.73	0.53
2:B:2121:THR:HB	6:B:2267:HOH:O	2.08	0.53
1:A:214:MET:SD	1:A:214:MET:N	2.80	0.53
2:B:1577:VAL:HG13	2:B:1703:LEU:HG	1.90	0.53
2:B:2077:ASN:O	2:B:2167:TRP:HH2	1.90	0.53
1:A:13:ILE:O	1:A:13:ILE:HG13	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1810:GLU:O	2:B:1815:GLN:HA	2.08	0.53
2:B:1723:VAL:O	2:B:1724:ASP:C	2.51	0.53
1:A:232:MET:O	1:A:233:SER:HB2	2.08	0.53
2:B:1926:MET:C	2:B:1928:LYS:H	2.16	0.53
2:B:2062:LEU:O	2:B:2063:ASN:HB2	2.09	0.53
1:A:183:HIS:O	1:A:228:HIS:HB2	2.09	0.53
1:A:261:VAL:HG23	1:A:264:THR:CG2	2.38	0.53
2:B:1912:LEU:HB3	2:B:2011:PRO:HG2	1.91	0.53
1:A:233:SER:HB2	1:A:239:PHE:HZ	1.74	0.52
1:A:36:ILE:HG12	1:A:156:SER:OG	2.08	0.52
2:B:2054:TYR:N	2:B:2054:TYR:CD1	2.77	0.52
2:B:2086:LEU:CD1	2:B:2092:ILE:HD11	2.39	0.52
1:A:214:MET:HE1	1:A:295:TYR:CD2	2.44	0.52
2:B:1699:ILE:HG22	2:B:1733:MET:HE1	1.90	0.52
2:B:2109:VAL:CG2	2:B:2173:LEU:HG	2.39	0.52
1:A:47:LYS:HG2	1:A:48:GLU:N	2.25	0.52
1:A:212:GLY:C	1:A:214:MET:SD	2.93	0.52
2:B:1809:LEU:O	2:B:1831:LEU:HB2	2.10	0.52
1:A:250:GLN:CD	1:A:255:ILE:HD13	2.34	0.52
2:B:1835:ALA:HB1	2:B:1861:ILE:HD13	1.92	0.52
2:B:1887:PHE:CE2	2:B:1892:GLU:HG2	2.44	0.52
1:A:69:ILE:O	1:A:69:ILE:HG22	2.09	0.52
2:B:2039:LYS:HZ3	2:B:2039:LYS:N	2.08	0.52
1:A:56:GLY:HA3	1:A:207:ASN:O	2.10	0.52
1:A:143:ILE:C	1:A:143:ILE:HD12	2.34	0.52
1:A:196:TRP:HE3	1:A:196:TRP:HA	1.75	0.52
1:A:212:GLY:O	1:A:214:MET:HG3	2.09	0.52
2:B:1551:GLU:OE2	2:B:1741:TRP:HH2	1.92	0.52
2:B:1959:ASP:O	2:B:1960:ARG:HB2	2.09	0.52
1:A:87:GLN:HG2	1:A:143:ILE:HG13	1.91	0.52
2:B:1610:GLU:HA	2:B:1710:CYS:O	2.10	0.52
2:B:1899:ASN:O	2:B:1900:ASN:C	2.53	0.52
1:A:132:PRO:HB2	1:A:166:LYS:HE2	1.90	0.51
2:B:1905:ASN:O	2:B:2014:ARG:HD3	2.10	0.51
1:A:37:VAL:HG12	1:A:38:TYR:N	2.24	0.51
2:B:2125:PRO:O	2:B:2127:ARG:HG3	2.10	0.51
1:A:49:LYS:O	1:A:50:PRO:O	2.29	0.51
1:A:58:LEU:HD11	1:A:161:PRO:HD3	1.92	0.51
1:A:196:TRP:HA	1:A:196:TRP:CE3	2.45	0.51
1:A:206:VAL:O	1:A:207:ASN:CB	2.58	0.51
2:B:2086:LEU:HD13	2:B:2092:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2106:GLU:CD	2:B:2143:VAL:HG21	2.36	0.51
1:A:187:PHE:CE2	1:A:241:ILE:HG12	2.45	0.51
2:B:2069:ASN:O	2:B:2070:ALA:HB2	2.11	0.51
3:B:2187:NAG:O3	3:B:2187:NAG:H83	2.11	0.51
2:B:1714:THR:O	2:B:1722:PRO:CD	2.59	0.51
2:B:1960:ARG:HD2	2:B:1960:ARG:O	2.10	0.51
2:B:1991:ILE:O	2:B:1991:ILE:HG22	2.11	0.51
2:B:1664:THR:HG22	2:B:1665:TYR:N	2.24	0.51
2:B:1781:GLU:OE2	2:B:1864:ARG:HB2	2.10	0.51
2:B:2083:GLN:HB3	2:B:2161:ARG:CG	2.38	0.51
1:A:167:LYS:H	1:A:167:LYS:CD	2.21	0.51
1:A:177:LYS:HG2	1:A:178:MET:N	2.26	0.51
2:B:1679:ASN:HB2	2:B:1680:PRO:HD3	1.93	0.51
2:B:1818:LEU:N	2:B:1818:LEU:HD22	2.25	0.51
2:B:1912:LEU:C	2:B:1914:THR:N	2.69	0.51
1:A:90:LYS:HD2	1:A:130:SER:HB3	1.92	0.50
2:B:2038:ASN:O	2:B:2040:GLN:N	2.41	0.50
2:B:1618:ARG:HH11	2:B:1664:THR:HG21	1.77	0.50
2:B:2086:LEU:O	2:B:2088:LYS:N	2.44	0.50
2:B:1731:LEU:HB2	2:B:1790:LEU:CD1	2.42	0.50
2:B:1789:LEU:HD12	2:B:1831:LEU:HD21	1.92	0.50
2:B:1965:ILE:HG21	2:B:1974:VAL:HG11	1.93	0.50
1:A:165:CYS:SG	1:A:170:LEU:HD13	2.51	0.50
2:B:1789:LEU:CD1	2:B:1831:LEU:HD21	2.42	0.50
2:B:1917:ASN:ND2	2:B:1919:GLU:HB2	2.24	0.50
1:A:177:LYS:O	1:A:179:PHE:N	2.44	0.50
2:B:1784:TRP:CD2	3:B:2188:NAG:H81	2.46	0.50
1:A:105:LEU:HB3	1:A:106:PRO:HD2	1.94	0.50
2:B:1557:SER:O	2:B:1558:LYS:C	2.53	0.49
2:B:2048:LYS:HG2	2:B:2054:TYR:CD2	2.47	0.49
1:A:180:GLU:OE1	1:A:181:LYS:HB2	2.12	0.49
2:B:1931:LEU:O	2:B:2019:GLY:HA3	2.12	0.49
2:B:1770:MET:HE2	2:B:1774:LEU:HD12	1.95	0.49
2:B:1575:LYS:HE2	2:B:1741:TRP:CE3	2.48	0.49
2:B:1730:LEU:HD22	2:B:1730:LEU:N	2.27	0.49
2:B:1723:VAL:HG12	2:B:1724:ASP:N	2.28	0.49
2:B:1812:GLY:C	2:B:1814:GLN:N	2.69	0.49
1:A:83:SER:HB3	1:A:112:ASP:O	2.13	0.49
1:A:247:VAL:HG22	1:A:247:VAL:O	2.12	0.49
2:B:1657:ASN:HD22	2:B:1658:ALA:N	2.11	0.49
2:B:1740:SER:OG	2:B:1741:TRP:CD1	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1550:GLU:OE2	2:B:1582:TYR:HE1	1.96	0.49
2:B:1617:VAL:HG21	2:B:1629:LEU:HD13	1.94	0.49
2:B:1870:MET:HG2	2:B:1926:MET:CE	2.43	0.49
2:B:1935:ILE:HD11	2:B:2002:ILE:HD13	1.95	0.49
1:A:37:VAL:CG1	1:A:39:ARG:HH11	2.24	0.48
2:B:1919:GLU:HB3	2:B:1920:PRO:HD3	1.95	0.48
1:A:126:ILE:HG13	1:A:126:ILE:O	2.12	0.48
1:A:186:MET:HE3	1:A:188:ALA:CB	2.43	0.48
1:A:36:ILE:N	1:A:156:SER:O	2.39	0.48
1:A:229:LEU:HD23	1:A:241:ILE:CD1	2.32	0.48
2:B:1554:TRP:O	2:B:1573:VAL:HA	2.13	0.48
1:A:147:TYR:O	1:A:149:ASN:N	2.47	0.48
1:A:152:GLU:O	1:A:153:ASP:C	2.56	0.48
1:A:189:VAL:HB	1:A:204:TYR:CD1	2.48	0.48
2:B:1590:LEU:O	2:B:1592:PRO:HD3	2.14	0.48
1:A:125:ILE:O	1:A:125:ILE:HG22	2.12	0.48
2:B:1540:GLY:HA2	2:B:1612:ASP:O	2.13	0.48
2:B:1574:TYR:CD1	2:B:1737:GLU:HG3	2.48	0.48
2:B:1742:TYR:O	2:B:1744:ASP:N	2.46	0.48
2:B:1843:LEU:O	2:B:1856:GLN:HA	2.12	0.48
2:B:1914:THR:CB	2:B:1920:PRO:HD2	2.27	0.48
1:A:179:PHE:O	1:A:180:GLU:O	2.32	0.48
1:A:233:SER:O	1:A:235:GLY:N	2.43	0.48
1:A:161:PRO:HG3	1:A:230:ILE:HD12	1.94	0.48
2:B:1821:TRP:CZ3	2:B:1823:LEU:HA	2.49	0.48
2:B:1914:THR:HB	2:B:1920:PRO:CD	2.27	0.48
2:B:2099:GLY:HA3	2:B:2108:TYR:HB3	1.96	0.48
1:A:248:LEU:HD23	1:A:248:LEU:H	1.78	0.48
2:B:1716:ASP:O	2:B:1719:THR:N	2.47	0.48
1:A:145:TYR:HE2	1:A:150:LEU:HD22	1.79	0.48
1:A:282:SER:O	1:A:284:ILE:N	2.47	0.48
2:B:1550:GLU:OE2	2:B:1582:TYR:CE1	2.67	0.47
1:A:47:LYS:HG2	1:A:48:GLU:H	1.78	0.47
2:B:1804:HIS:O	2:B:1806:GLN:HG2	2.15	0.47
2:B:1898:LEU:O	2:B:1899:ASN:HB2	2.14	0.47
2:B:2049:SER:C	2:B:2051:TRP:H	2.22	0.47
2:B:1831:LEU:N	2:B:1831:LEU:HD23	2.29	0.47
2:B:2049:SER:HB2	2:B:2051:TRP:CZ3	2.49	0.47
2:B:1787:LEU:HD21	2:B:1833:MET:HB3	1.95	0.47
2:B:2076:ASN:HD22	2:B:2076:ASN:N	2.12	0.47
1:A:53:ARG:HH22	1:A:217:ILE:HG12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1710:CYS:SG	2:B:1715:LEU:HD21	2.54	0.47
2:B:1854:GLY:O	2:B:1856:GLN:N	2.46	0.47
2:B:2168:ASN:C	2:B:2168:ASN:ND2	2.63	0.47
1:A:87:GLN:O	1:A:87:GLN:CG	2.62	0.47
1:A:149:ASN:HD22	1:A:150:LEU:N	2.12	0.47
2:B:1576:LYS:HD2	2:B:1701:SER:O	2.14	0.47
2:B:1797:ASP:O	2:B:1798:ILE:O	2.33	0.47
2:B:1844:ASP:HB2	2:B:1851:GLN:CG	2.45	0.47
2:B:2121:THR:O	2:B:2122:ASP:HB2	2.14	0.47
2:B:2162:ILE:N	2:B:2162:ILE:CD1	2.69	0.47
1:A:191:ASP:C	1:A:191:ASP:OD2	2.57	0.47
2:B:1618:ARG:HD2	2:B:1664:THR:CG2	2.45	0.47
2:B:1629:LEU:CD2	2:B:1669:TRP:HH2	2.27	0.47
2:B:1716:ASP:O	2:B:1717:LYS:C	2.58	0.47
1:A:65:GLU:HB2	1:A:68:ASP:OD1	2.14	0.47
1:A:147:TYR:CD1	1:A:150:LEU:HD21	2.50	0.47
2:B:1771:ILE:HG13	2:B:1771:ILE:O	2.15	0.47
2:B:1905:ASN:HD22	2:B:1905:ASN:N	1.99	0.47
2:B:1802:HIS:HB3	2:B:1844:ASP:OD1	2.14	0.46
2:B:2044:SER:HB3	2:B:2081:TRP:CE2	2.50	0.46
1:A:133:THR:H	1:A:136:ASP:CG	2.23	0.46
1:A:81:PRO:O	1:A:82:LEU:HD23	2.15	0.46
1:A:161:PRO:HG3	1:A:230:ILE:HD11	1.98	0.46
2:B:2110:LYS:CB	2:B:2166:THR:HG23	2.44	0.46
2:B:2047:LYS:O	2:B:2048:LYS:HG3	2.15	0.46
2:B:2046:PHE:HA	2:B:2072:GLN:O	2.15	0.46
2:B:2034:GLY:O	2:B:2035:LYS:C	2.59	0.46
2:B:2085:ASP:C	2:B:2087:LEU:H	2.22	0.46
2:B:1539:THR:O	2:B:1541:ASN:N	2.48	0.46
2:B:1599:HIS:NE2	2:B:1728:PHE:HD1	2.14	0.46
2:B:1692:ALA:O	2:B:1693:VAL:C	2.59	0.46
2:B:1714:THR:O	2:B:1722:PRO:HD2	2.14	0.46
2:B:1722:PRO:HG2	2:B:1723:VAL:H	1.80	0.46
2:B:1724:ASP:C	2:B:1725:MET:O	2.58	0.46
1:A:136:ASP:HB2	1:A:137:PRO:HD2	1.97	0.46
2:B:1557:SER:O	2:B:1560:VAL:HG12	2.15	0.46
2:B:1814:GLN:HG2	2:B:1816:HIS:NE2	2.31	0.46
2:B:2068:VAL:HG23	2:B:2068:VAL:O	2.16	0.46
1:A:205:THR:O	1:A:206:VAL:HG23	2.16	0.46
2:B:1770:MET:CE	2:B:1774:LEU:HD12	2.46	0.46
2:B:1893:PRO:C	2:B:1895:LEU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HD12	1:A:78:ALA:HB1	1.98	0.46
2:B:1851:GLN:HE21	2:B:1851:GLN:C	2.24	0.46
2:B:1872:LEU:HG	2:B:1877:ILE:HD12	1.98	0.46
1:A:243:PHE:CE1	1:A:280:ILE:HD13	2.51	0.45
2:B:1724:ASP:OD2	2:B:1786:ARG:HB2	2.16	0.45
2:B:2055:TRP:CG	2:B:2072:GLN:HB2	2.50	0.45
1:A:71:LYS:NZ	1:A:71:LYS:CB	2.79	0.45
1:A:169:THR:O	1:A:177:LYS:HB2	2.15	0.45
2:B:1539:THR:OG1	2:B:1712:LYS:NZ	2.49	0.45
2:B:1694:ASN:O	2:B:1695:PRO:C	2.58	0.45
2:B:2050:TRP:H	2:B:2050:TRP:HE3	1.63	0.45
2:B:1583:LEU:HD21	2:B:1973:ASN:HD21	1.81	0.45
2:B:1836:SER:O	2:B:1837:LYS:HB2	2.15	0.45
2:B:2151:PHE:O	2:B:2152:ASN:C	2.58	0.45
1:A:80:LYS:HZ3	1:A:152:GLU:HG2	1.78	0.45
2:B:1803:PHE:CD1	2:B:1843:LEU:HD13	2.52	0.45
2:B:1942:HIS:ND1	2:B:1943:TYR:HD1	2.14	0.45
1:A:59:GLY:O	1:A:60:PRO:O	2.35	0.45
1:A:187:PHE:HD1	1:A:187:PHE:H	1.65	0.45
1:A:239:PHE:HD1	1:A:287:HIS:CE1	2.34	0.45
2:B:1870:MET:HG3	6:B:2199:HOH:O	2.16	0.45
1:A:129:HIS:ND1	1:A:129:HIS:C	2.75	0.45
2:B:1632:HIS:HB3	2:B:1688:ALA:O	2.16	0.45
2:B:1657:ASN:C	2:B:1657:ASN:ND2	2.70	0.45
2:B:1791:ASN:HB2	2:B:1823:LEU:HD13	1.98	0.45
2:B:1801:VAL:O	2:B:1801:VAL:HG23	2.14	0.45
2:B:1939:GLY:O	2:B:2014:ARG:NE	2.46	0.45
2:B:2049:SER:OG	2:B:2053:ASN:HB2	2.16	0.45
1:A:255:ILE:HD12	1:A:257:ALA:O	2.16	0.45
2:B:1611:VAL:O	2:B:1612:ASP:HB2	2.16	0.45
2:B:2058:PHE:CD1	2:B:2058:PHE:C	2.95	0.45
2:B:2140:ASN:HA	2:B:2147:VAL:HG21	1.99	0.45
1:A:238:LEU:HD23	1:A:238:LEU:N	2.32	0.45
2:B:1631:ALA:HB2	2:B:1669:TRP:CZ2	2.52	0.45
2:B:1969:ASN:CG	3:B:2189:NAG:HN2	2.21	0.45
1:A:10:ALA:O	1:A:77:LYS:HB2	2.17	0.44
1:A:89:ILE:HD11	1:A:164:ILE:HD11	1.99	0.44
2:B:1618:ARG:HD2	2:B:1664:THR:HG22	1.99	0.44
2:B:1893:PRO:C	2:B:1895:LEU:N	2.75	0.44
1:A:229:LEU:N	1:A:229:LEU:CD1	2.80	0.44
1:A:261:VAL:HG23	1:A:264:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2015:LEU:C	2:B:2015:LEU:HD12	2.41	0.44
1:A:133:THR:HG21	2:B:1815:GLN:HB2	1.99	0.44
2:B:1716:ASP:O	2:B:1718:GLU:N	2.50	0.44
2:B:1726:ARG:HA	2:B:1726:ARG:HD3	1.62	0.44
2:B:1704:ILE:HD11	2:B:1792:LEU:HD12	1.99	0.44
2:B:1871:GLY:HA3	2:B:1876:LEU:HB2	2.00	0.44
2:B:1991:ILE:O	2:B:1992:ASP:C	2.60	0.44
2:B:2123:TRP:CZ3	2:B:2161:ARG:HG3	2.53	0.44
2:B:1925:ASP:OD1	2:B:1925:ASP:C	2.60	0.44
2:B:2000:ILE:HG13	2:B:2017:LEU:HD13	1.99	0.44
1:A:108:GLU:O	1:A:111:ASP:OD1	2.35	0.44
1:A:144:TYR:CD1	1:A:144:TYR:C	2.96	0.44
1:A:219:VAL:HG12	1:A:220:CYS:N	2.32	0.44
2:B:1686:ALA:HA	2:B:1708:LEU:HD12	2.00	0.44
1:A:35:LYS:NZ	1:A:192:GLU:OE1	2.46	0.44
1:A:161:PRO:CG	1:A:184:VAL:HG11	2.43	0.44
2:B:1832:GLU:HG3	3:B:2188:NAG:O7	2.17	0.44
2:B:2067:ARG:HH11	2:B:2067:ARG:CA	2.17	0.44
1:A:54:THR:O	1:A:55:SER:C	2.61	0.44
2:B:2092:ILE:HG22	2:B:2151:PHE:CE2	2.48	0.44
2:B:2112:TYR:N	2:B:2112:TYR:HD2	2.16	0.44
1:A:204:TYR:HB3	1:A:292:MET:SD	2.57	0.43
2:B:1790:LEU:O	2:B:1790:LEU:HD12	2.18	0.43
2:B:1900:ASN:OD1	2:B:1905:ASN:HB2	2.18	0.43
2:B:1939:GLY:O	2:B:2014:ARG:NH2	2.50	0.43
2:B:1926:MET:O	2:B:1927:GLN:HB2	2.18	0.43
1:A:136:ASP:OD2	1:A:140:LEU:HD21	2.18	0.43
1:A:284:ILE:C	1:A:286:ARG:H	2.27	0.43
2:B:1722:PRO:HG2	2:B:1723:VAL:N	2.32	0.43
2:B:1723:VAL:C	2:B:1725:MET:N	2.73	0.43
1:A:87:GLN:CG	1:A:143:ILE:HG13	2.49	0.43
1:A:133:THR:CG2	1:A:134:HIS:H	2.22	0.43
1:A:163:LEU:HD22	1:A:228:HIS:CE1	2.53	0.43
1:A:209:TYR:CD2	1:A:214:MET:HB3	2.53	0.43
2:B:1612:ASP:HB2	2:B:1712:LYS:HZ1	1.82	0.43
2:B:1872:LEU:HB2	2:B:2016:GLU:OE2	2.18	0.43
2:B:1950:THR:O	2:B:1951:GLU:HB2	2.18	0.43
1:A:143:ILE:HD12	1:A:144:TYR:N	2.34	0.43
2:B:1944:LEU:O	2:B:1946:PRO:HD3	2.19	0.43
2:B:2070:ALA:HB1	2:B:2173:LEU:O	2.18	0.43
1:A:146:SER:CB	1:A:153:ASP:OD1	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HE3	1:A:293:GLN:O	2.18	0.43
2:B:1894:LYS:N	2:B:1894:LYS:CD	2.82	0.43
2:B:2162:ILE:HD12	2:B:2162:ILE:H	1.79	0.43
1:A:48:GLU:CD	1:A:50:PRO:HG3	2.43	0.42
1:A:133:THR:HB	1:A:136:ASP:OD1	2.19	0.42
1:A:276:GLY:O	1:A:277:ARG:HG2	2.19	0.42
2:B:1706:PRO:CB	2:B:1729:VAL:HG11	2.47	0.42
2:B:2054:TYR:O	2:B:2068:VAL:HG21	2.18	0.42
2:B:2098:GLN:HA	2:B:2140:ASN:ND2	2.34	0.42
1:A:39:ARG:HB3	1:A:48:GLU:OE2	2.19	0.42
2:B:1914:THR:HG21	2:B:2004:PRO:O	2.19	0.42
2:B:1621:ASN:OD1	2:B:1621:ASN:C	2.62	0.42
2:B:1935:ILE:HD11	2:B:2002:ILE:CD1	2.49	0.42
2:B:2016:GLU:OE2	2:B:2016:GLU:HA	2.18	0.42
1:A:154:PHE:CD1	1:A:232:MET:HG2	2.55	0.42
2:B:1736:ASP:C	2:B:1738:LYS:N	2.78	0.42
2:B:1876:LEU:HD22	2:B:2148:LYS:HB2	2.01	0.42
2:B:2038:ASN:C	2:B:2040:GLN:N	2.77	0.42
1:A:181:LYS:HA	6:A:2276:HOH:O	2.20	0.42
2:B:1967:LYS:HG2	2:B:1968:GLY:N	2.34	0.42
1:A:248:LEU:HG	1:A:248:LEU:O	2.18	0.42
1:A:280:ILE:HB	1:A:294:ALA:O	2.20	0.42
1:A:287:HIS:O	1:A:292:MET:HB2	2.19	0.42
2:B:1594:GLY:H	2:B:1596:TYR:HE2	1.68	0.42
2:B:1711:ARG:O	2:B:1712:LYS:C	2.62	0.42
2:B:2155:ILE:HG21	2:B:2160:ILE:HD11	2.02	0.42
1:A:48:GLU:C	1:A:50:PRO:HD3	2.44	0.42
1:A:83:SER:HB2	1:A:122:TYR:OH	2.20	0.42
2:B:1555:ASP:C	2:B:1556:TYR:O	2.60	0.42
2:B:1557:SER:O	2:B:1560:VAL:N	2.50	0.42
2:B:1741:TRP:O	2:B:1742:TYR:C	2.62	0.42
2:B:1784:TRP:CZ2	2:B:1834:LYS:HB2	2.55	0.42
2:B:1817:GLN:HA	2:B:1817:GLN:NE2	2.33	0.42
2:B:1895:LEU:O	2:B:1897:ARG:N	2.51	0.42
2:B:1927:GLN:CA	2:B:1998:ARG:HE	2.32	0.42
2:B:2081:TRP:HZ3	2:B:2083:GLN:HG2	1.82	0.42
1:A:15:TRP:CH2	1:A:208:GLY:HA3	2.55	0.42
2:B:1632:HIS:HB2	2:B:1690:TYR:CE1	2.55	0.42
2:B:1721:MET:HE3	2:B:1786:ARG:NH1	2.19	0.42
2:B:1969:ASN:OD1	3:B:2189:NAG:H3	2.19	0.42
2:B:2037:GLU:HB3	2:B:2039:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2167:TRP:CE3	2:B:2171:ILE:HD11	2.55	0.42
1:A:171:THR:HG22	1:A:172:GLU:N	2.34	0.41
2:B:1714:THR:O	2:B:1722:PRO:HD3	2.20	0.41
2:B:1913:SER:O	2:B:1915:GLU:OE2	2.38	0.41
2:B:2044:SER:HB3	2:B:2081:TRP:NE1	2.35	0.41
2:B:2101:LYS:CD	2:B:2144:ARG:NH2	2.81	0.41
1:A:53:ARG:HG3	1:A:53:ARG:O	2.20	0.41
1:A:153:ASP:HA	1:A:158:LEU:HD12	2.02	0.41
2:B:1618:ARG:HD3	2:B:1666:THR:OG1	2.19	0.41
1:A:144:TYR:C	1:A:145:TYR:HD1	2.28	0.41
2:B:1680:PRO:HB2	2:B:1812:GLY:C	2.46	0.41
2:B:1802:HIS:N	2:B:1844:ASP:O	2.47	0.41
1:A:16:ASN:O	1:A:16:ASN:CG	2.63	0.41
1:A:160:GLY:HA2	1:A:161:PRO:HD3	1.84	0.41
2:B:1662:ASN:CB	3:B:2187:NAG:H5	2.49	0.41
1:A:66:VAL:O	1:A:66:VAL:HG23	2.20	0.41
1:A:89:ILE:CG2	1:A:90:LYS:N	2.83	0.41
1:A:254:LYS:HD3	1:A:254:LYS:O	2.21	0.41
2:B:1813:THR:HG22	2:B:1813:THR:O	2.21	0.41
1:A:191:ASP:OD2	1:A:193:SER:CB	2.69	0.41
1:A:216:ASP:HB3	1:A:295:TYR:O	2.21	0.41
2:B:1820:VAL:HG11	2:B:1846:GLU:OE2	2.20	0.41
2:B:1998:ARG:NH1	2:B:1999:TYR:OH	2.54	0.41
1:A:176:GLN:HB3	1:A:180:GLU:HA	2.02	0.41
1:A:179:PHE:N	1:A:179:PHE:CD1	2.89	0.41
2:B:1557:SER:HB3	2:B:1771:ILE:HD11	2.01	0.41
2:B:1578:VAL:HA	2:B:1703:LEU:HD23	2.03	0.41
2:B:1740:SER:OG	2:B:1741:TRP:HD1	2.04	0.41
1:A:135:ASP:OD1	1:A:135:ASP:O	2.39	0.41
1:A:147:TYR:C	1:A:149:ASN:N	2.78	0.41
2:B:1704:ILE:HG12	2:B:1705:GLY:N	2.36	0.41
2:B:1817:GLN:HE21	2:B:1817:GLN:CA	2.32	0.41
2:B:1818:LEU:N	2:B:1818:LEU:CD2	2.84	0.41
1:A:12:SER:HA	1:A:35:LYS:O	2.21	0.41
2:B:1914:THR:CG2	2:B:2004:PRO:O	2.69	0.41
1:A:31:THR:HB	1:A:32:SER:H	1.67	0.40
1:A:202:LEU:HD23	1:A:203:MET:N	2.30	0.40
2:B:1737:GLU:C	2:B:1739:LYS:H	2.28	0.40
2:B:1886:GLU:OE1	2:B:1911:LYS:HE3	2.20	0.40
2:B:1894:LYS:H	2:B:1894:LYS:CD	2.35	0.40
2:B:2003:SER:HA	2:B:2004:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2057:PRO:C	2:B:2059:LEU:H	2.29	0.40
2:B:2083:GLN:HA	2:B:2160:ILE:O	2.21	0.40
2:B:2089:ILE:HD11	2:B:2118:ASP:OD2	2.21	0.40
1:A:36:ILE:O	1:A:156:SER:O	2.39	0.40
1:A:37:VAL:CG1	1:A:38:TYR:N	2.83	0.40
1:A:55:SER:O	1:A:56:GLY:O	2.40	0.40
1:A:133:THR:N	1:A:136:ASP:OD1	2.55	0.40
1:A:192:GLU:HB3	1:A:199:THR:OG1	2.22	0.40
2:B:1789:LEU:HD13	2:B:1801:VAL:HG21	2.03	0.40
2:B:1912:LEU:C	2:B:1912:LEU:HD12	2.46	0.40
2:B:1557:SER:O	2:B:1559:PHE:N	2.55	0.40
2:B:2045:SER:HB2	2:B:2074:LYS:HB3	2.02	0.40
1:A:15:TRP:O	1:A:32:SER:HA	2.20	0.40
1:A:64:ALA:CB	1:A:70:MET:HE2	2.51	0.40
1:A:155:ASN:C	1:A:157:GLY:N	2.75	0.40
1:A:175:THR:HG22	1:A:176:GLN:N	2.36	0.40
2:B:2031:MET:HE1	2:B:2041:ILE:HD13	2.03	0.40
1:A:244:ASN:HB3	1:A:278:TRP:CE3	2.56	0.40
2:B:1770:MET:HG2	2:B:1773:ASN:O	2.22	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	260/306 (85%)	178 (68%)	46 (18%)	36 (14%)	0	0
2	B	593/647 (92%)	479 (81%)	73 (12%)	41 (7%)	1	2
All	All	853/953 (90%)	657 (77%)	119 (14%)	77 (9%)	0	1

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	60	PRO
1	A	180	GLU
1	A	187	PHE
1	A	206	VAL
1	A	207	ASN
1	A	210	VAL
1	A	233	SER
1	A	262	SER
1	A	285	PRO
2	B	1680	PRO
2	B	1682	SER
2	B	1723	VAL
2	B	1725	MET
2	B	1867	LYS
2	B	1970	SER
2	B	2050	TRP
2	B	2067	ARG
1	A	56	GLY
1	A	61	THR
1	A	159	ILE
1	A	178	MET
1	A	246	GLN
1	A	283	LEU
2	B	1540	GLY
2	B	1558	LYS
2	B	1662	ASN
2	B	1671	ALA
2	B	1695	PRO
2	B	1717	LYS
2	B	1719	THR
2	B	1848	GLY
2	B	1889	GLY
2	B	1913	SER
2	B	2039	LYS
2	B	2087	LEU
1	A	53	ARG
1	A	88	GLY
1	A	148	VAL
1	A	153	ASP
1	A	203	MET
1	A	216	ASP
2	B	1634	LEU

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Mol	Chain	Res	Type
2	B	1665	TYR
2	B	1722	PRO
2	B	1794	GLY
2	B	1846	GLU
2	B	1896	ALA
2	B	2078	ASN
1	A	2	LYS
1	A	41	TYR
1	A	43	ALA
1	A	116	PRO
1	A	156	SER
1	A	195	SER
1	A	215	PRO
2	B	1712	LYS
2	B	1797	ASP
2	B	1798	ILE
2	B	1837	LYS
2	B	1918	PRO
2	B	1993	PRO
2	B	2122	ASP
1	A	152	GLU
1	A	177	LYS
1	A	234	SER
2	B	1557	SER
2	B	1914	THR
2	B	2009	ASN
1	A	45	PHE
1	A	137	PRO
2	B	1743	TYR
2	B	1942	HIS
2	B	1960	ARG
1	A	217	ILE
2	B	1661	PRO
1	A	126	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/269 (87%)	205 (88%)	28 (12%)	5	17
2	B	526/570 (92%)	469 (89%)	57 (11%)	6	21
All	All	759/839 (90%)	674 (89%)	85 (11%)	6	19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	8	VAL
1	A	40	GLU
1	A	46	GLN
1	A	54	THR
1	A	71	LYS
1	A	87	GLN
1	A	94	PHE
1	A	120	TYR
1	A	126	ILE
1	A	129	HIS
1	A	143	ILE
1	A	145	TYR
1	A	152	GLU
1	A	176	GLN
1	A	180	GLU
1	A	183	HIS
1	A	189	VAL
1	A	196	TRP
1	A	203	MET
1	A	211	ASN
1	A	214	MET
1	A	243	PHE
1	A	254	LYS
1	A	261	VAL
1	A	267	THR
1	A	283	LEU
1	A	285	PRO
2	B	1539	THR
2	B	1542	ARG
2	B	1573	VAL
2	B	1580	ARG
2	B	1596	TYR
2	B	1600	LEU
2	B	1606	VAL

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Mol	Chain	Res	Type
2	B	1613	ASP
2	B	1617	VAL
2	B	1657	ASN
2	B	1660	GLN
2	B	1696	GLU
2	B	1704	ILE
2	B	1707	LEU
2	B	1708	LEU
2	B	1711	ARG
2	B	1717	LYS
2	B	1718	GLU
2	B	1720	ASN
2	B	1726	ARG
2	B	1790	LEU
2	B	1797	ASP
2	B	1808	LEU
2	B	1823	LEU
2	B	1831	LEU
2	B	1832	GLU
2	B	1845	THR
2	B	1851	GLN
2	B	1852	ARG
2	B	1887	PHE
2	B	1890	TYR
2	B	1895	LEU
2	B	1898	LEU
2	B	1900	ASN
2	B	1905	ASN
2	B	1914	THR
2	B	1915	GLU
2	B	1918	PRO
2	B	1928	LYS
2	B	1931	LEU
2	B	1991	ILE
2	B	2039	LYS
2	B	2054	TYR
2	B	2067	ARG
2	B	2089	ILE
2	B	2093	THR
2	B	2097	THR
2	B	2112	TYR
2	B	2113	THR

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Mol	Chain	Res	Type
2	B	2128	GLU
2	B	2132	MET
2	B	2140	ASN
2	B	2141	ASN
2	B	2143	VAL
2	B	2162	ILE
2	B	2168	ASN
2	B	2175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	11	GLN
1	A	73	HIS
1	A	85	HIS
1	A	103	HIS
1	A	142	HIS
1	A	149	ASN
1	A	155	ASN
1	A	182	GLN
1	A	242	HIS
2	B	1657	ASN
2	B	1694	ASN
2	B	1782	GLN
2	B	1804	HIS
2	B	1815	GLN
2	B	1817	GLN
2	B	1851	GLN
2	B	1905	ASN
2	B	1927	GLN
2	B	1936	GLN
2	B	2009	ASN
2	B	2018	GLN
2	B	2023	ASN
2	B	2065	GLN
2	B	2076	ASN
2	B	2078	ASN
2	B	2079	ASN
2	B	2168	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2188	2	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
3	NAG	A	2186	1	14,14,15	0.53	0	17,19,21	0.70	0
3	NAG	B	2187	2	14,14,15	0.61	0	17,19,21	0.79	0
3	NAG	B	2189	2	14,14,15	0.66	0	17,19,21	0.68	0
3	NAG	A	2185	1	14,14,15	0.67	0	17,19,21	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	2188	2	-	2/6/23/26	0/1/1/1
3	NAG	A	2186	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2187	2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	2189	2	1/1/5/7	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2185	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2188	NAG	C2-N2-C7	-2.21	119.94	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	2187	NAG	C1
3	B	2189	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2185	NAG	C8-C7-N2-C2
3	A	2185	NAG	O7-C7-N2-C2
3	A	2186	NAG	C8-C7-N2-C2
3	A	2186	NAG	O7-C7-N2-C2
3	B	2187	NAG	C8-C7-N2-C2
3	B	2187	NAG	O7-C7-N2-C2
3	B	2189	NAG	C4-C5-C6-O6
3	B	2189	NAG	O5-C5-C6-O6
3	A	2186	NAG	O5-C5-C6-O6
3	A	2186	NAG	C4-C5-C6-O6
3	B	2188	NAG	C8-C7-N2-C2
3	B	2188	NAG	O7-C7-N2-C2
3	A	2185	NAG	C4-C5-C6-O6
3	B	2187	NAG	C4-C5-C6-O6
3	B	2187	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2188	NAG	4	0
3	B	2187	NAG	4	0
3	B	2189	NAG	3	0
3	A	2185	NAG	3	0

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	268/306 (87%)	0.94	25 (9%)	14 10	48, 89, 127, 136	0
2	B	601/647 (92%)	0.10	14 (2%)	61 51	26, 54, 91, 112	0
All	All	869/953 (91%)	0.36	39 (4%)	38 30	26, 64, 116, 136	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	5.6
2	B	1721	MET	4.4
1	A	217	ILE	3.7
1	A	188	ALA	3.5
1	A	54	THR	3.4
1	A	218	THR	3.3
1	A	288	PHE	2.9
1	A	248	LEU	2.9
1	A	189	VAL	2.7
2	B	1793	GLY	2.7
1	A	290	ALA	2.7
2	B	1992	ASP	2.7
1	A	58	LEU	2.6
1	A	292	MET	2.6
2	B	2111	SER	2.6
1	A	43	ALA	2.6
2	B	1613	ASP	2.6
2	B	2050	TRP	2.5
1	A	283	LEU	2.5
1	A	38	TYR	2.5
2	B	1798	ILE	2.5
1	A	57	LEU	2.4
1	A	48	GLU	2.4
1	A	8	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	253	HIS	2.4
2	B	1692	ALA	2.3
1	A	55	SER	2.3
2	B	1846	GLU	2.2
1	A	41	TYR	2.2
2	B	1740	SER	2.2
2	B	2052	GLY	2.2
2	B	1684	CYS	2.2
2	B	2073	ALA	2.2
1	A	196	TRP	2.1
1	A	296	ILE	2.1
1	A	210	VAL	2.1
2	B	1725	MET	2.0
1	A	245	GLY	2.0
1	A	221	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	2185	14/15	0.28	0.14	127,128,129,130	0
3	NAG	B	2187	14/15	0.66	0.12	94,98,101,101	0
3	NAG	A	2186	14/15	0.80	0.12	86,88,90,91	0
3	NAG	B	2189	14/15	0.82	0.12	70,72,74,76	0
3	NAG	B	2188	14/15	0.88	0.10	73,74,76,78	0
4	CA	A	2184	1/1	0.92	0.07	68,68,68,68	0
5	CU	B	2190	1/1	0.96	0.09	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.