



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 PM UTC

PDB ID : 3H0J / pdb_00003h0j
Title : Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 2
Authors : Zhang, H.; Tong, L.
Deposited on : 2009-04-09
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

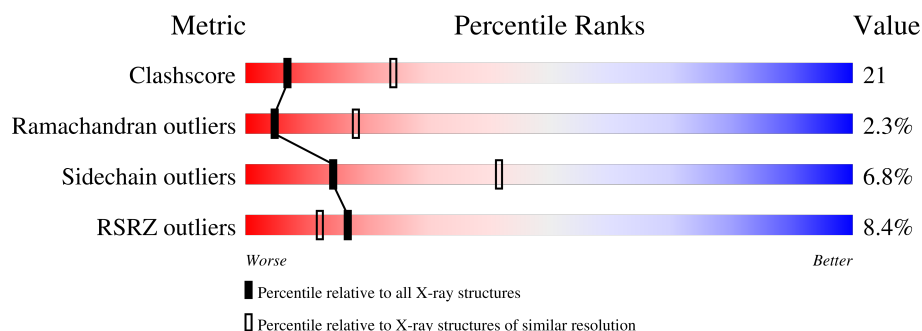
1 Overall quality at a glance

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))
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	769	5% 54% 29% 5% 11%
1	B	769	8% 47% 35% 6% 12%
1	C	769	9% 52% 29% 5% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16200 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	681	Total	C	N	O	S	0	0	0
			5424	3459	930	1016	19			
1	B	675	Total	C	N	O	S	0	0	0
			5376	3427	923	1007	19			
1	C	665	Total	C	N	O	S	0	0	0
			5298	3374	912	993	19			

There are 33 discrepancies between the modelled and reference sequences:

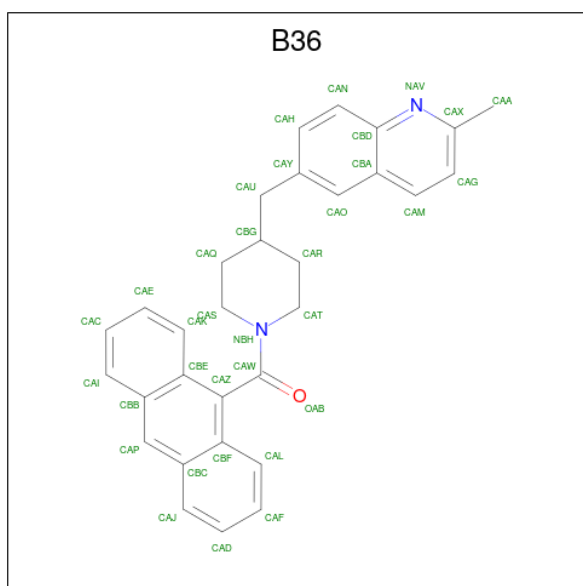
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	expression tag	UNP Q00955
A	1474	ALA	-	expression tag	UNP Q00955
A	1475	SER	-	expression tag	UNP Q00955
A	2234	LEU	-	expression tag	UNP Q00955
A	2235	GLU	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
A	2240	HIS	-	expression tag	UNP Q00955
A	2241	HIS	-	expression tag	UNP Q00955
B	1473	MET	-	expression tag	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	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
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	expression tag	UNP Q00955

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 6-[[1-(anthracen-9-ylcarbonyl)piperidin-4-yl]methyl]-2-methylquinoline (CCD ID: B36) (formula: C₃₁H₂₈N₂O).

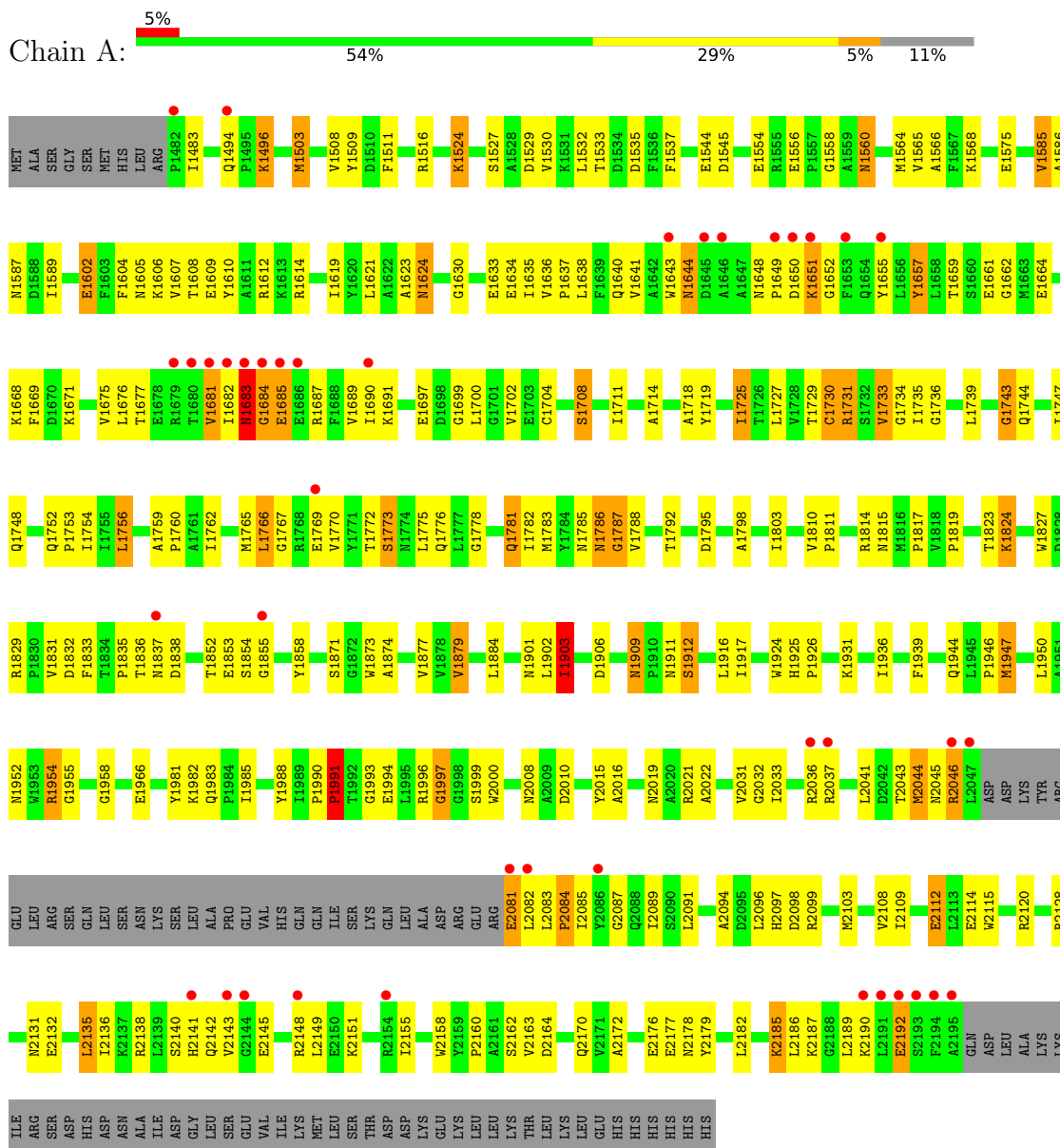


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	31	2	1		
2	B	1	Total	C	N	O	0	0
			34	31	2	1		
2	C	1	Total	C	N	O	0	0
			34	31	2	1		

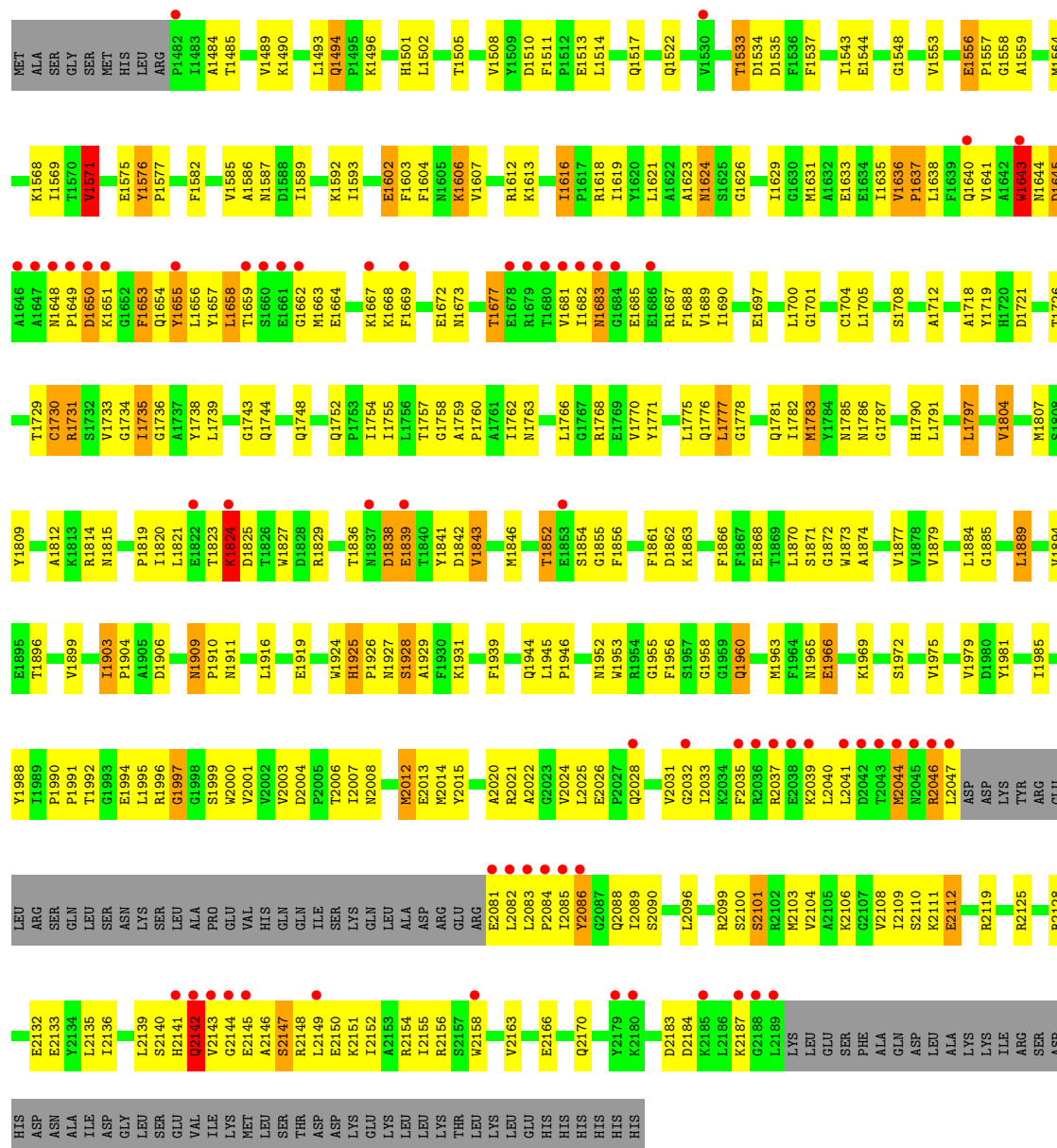
3 Residue-property plots

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: Acetyl-CoA carboxylase



- Molecule 1: Acetyl-CoA carboxylase



ALA	D2098	K2034	P1926	E1801	R1731	D1650
GLN	R2099	F2035	N1927	K1802	S1732	K1661
ASP	R2100	R2036	S1928	W1806	V1733	G1652
LEU	S2101	R2037	I1936	M1807	G1734	F1653
ALA	R2102	L2041	P1946	P1811	I1735	Q1654
LYS	M2103	R2042	L1950	R1814	G1736	Y1655
LYS	V2104	T2043	L1950	P1819	A1737	L1656
ILE	V2108	M2044	W1953	R1741	V1740	Y1657
ARG	I2109	R2045	R1954	L1742	L1742	L1658
SER	E2114	L2047	G1955	P1824	S1660	S1659
ASP	R2125	ASP	Q1960	R1829	E1661	E1661
ASN	R2128	LYS	M1963	I1837	G1662	G1662
ALA	R2129	TYR	E1966	R1844	M1663	M1663
ASP	E2132	ARG	Y1967	W1845	E1664	E1664
GLY	I2136	SER	L1968	M1846	T1665	T1665
LEU	L2139	LEU	A1977	I1847	L1666	L1666
SER	S2140	GLN	L1978	E1848	K1667	K1667
VAL	H2141	SER	K1982	G1849	K1668	K1668
LYS	Q2142	ASN	Y1988	R1850	F1669	F1669
MET	V2143	LYS	P1991	E1851	D1670	D1670
LEU	G2144	SER	T1992	T1852	K1671	K1671
THR	A2145	ALA	Y1988	W1853	V1675	V1675
ASP	E2146	PRO	P1990	S1854	L1676	L1676
ASP	S2147	GLU	P1991	Y1858	T1677	T1677
LYS	R2148	VAL	T1992	G1872	E1678	E1678
GLU	L2149	HIS	G1993	W1873	R1679	R1679
LYS	E2150	GLN	E1994	A1874	V1680	V1680
LEU	K2151	GLN	L1995	K1875	L1766	L1766
LEU	I2152	ILE	R1996	G1876	V1681	V1681
THR	A2153	SER	G1997	G1876	I1682	I1682
LEU	R2154	LYS	G1998	R1883	N1683	N1683
LYS	P2160	GLN	S1999	I1887	G1684	G1684
GLU	V2163	ALA	W2000	V1894	E1685	E1685
HIS	D2164	ASP	V2001	T1898	E1686	E1686
HIS	Q2170	ARG	D2004	V1899	R1687	R1687
HIS	T2173	ARG	P2005	T1898	F1688	F1688
HIS	E2177	ARG	M2008	V1899	Y1689	Y1689
	K2185	E2081	M2012	L1902	L1700	L1700
L2186	L2082	L2083	M2013	N1909	G1701	G1701
K2187	L2084	L2085	M2014	P1910	C1704	C1704
G2188	L2086	Y2086	Y2015	N1911	L1705	L1705
L2189	T2089	T2089	R2021	S1912	S1708	S1708
LYS	S2090	L2091	L2025	A1913	A1714	A1714
LEU	L2092	F2092	Q2028	E1914	T1715	T1715
LEU	F2093	L2096	V2031	E1919	Y1719	Y1719
GLU	H2097	H2097		W1924	T1725	T1725
SER				G1799	C1730	C1730
PHE				V1800		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.74Å 122.86Å 145.88Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	51.25 – 2.80 51.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.25-2.80) 99.2 (51.25-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.257 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	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	0.92	EDS
Total number of atoms	16200	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: B36

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	0.46	0/5546	1.01	31/7514 (0.4%)
1	B	0.45	0/5497	0.99	33/7449 (0.4%)
1	C	0.44	0/5415	0.97	24/7335 (0.3%)
All	All	0.45	0/16458	0.99	88/22298 (0.4%)

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1770	VAL	N-CA-C	11.04	121.89	110.62
1	A	2044	MET	N-CA-C	-9.30	101.94	113.20
1	C	1645	ASP	N-CA-C	-9.19	104.14	114.62
1	A	2046	ARG	N-CA-C	-8.63	100.73	112.03
1	B	1770	VAL	N-CA-C	8.22	118.25	110.53
1	C	1787	GLY	N-CA-C	-8.18	103.81	114.85
1	C	1785	ASN	N-CA-C	-8.05	102.09	112.23
1	A	1787	GLY	N-CA-C	-8.02	104.50	114.92
1	B	1712	ALA	N-CA-C	-7.33	102.89	111.03
1	A	1483	ILE	N-CA-C	7.15	118.29	110.21
1	B	1925	HIS	CA-C-N	-7.11	111.84	119.24
1	B	1925	HIS	C-N-CA	-7.11	111.84	119.24
1	C	1946	PRO	N-CA-C	-7.10	100.55	111.13
1	B	2044	MET	N-CA-C	-7.09	104.50	113.01
1	C	1648	ASN	CA-C-N	7.02	128.62	119.84
1	C	1648	ASN	C-N-CA	7.02	128.62	119.84
1	C	1624	ASN	N-CA-C	7.01	117.28	108.45
1	C	1909	ASN	CA-C-N	6.88	126.68	119.05
1	C	1909	ASN	C-N-CA	6.88	126.68	119.05
1	C	2046	ARG	N-CA-C	-6.74	103.14	112.30
1	B	1787	GLY	N-CA-C	-6.68	105.84	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1529	ASP	N-CA-C	6.63	118.30	111.14
1	B	1906	ASP	CA-C-N	6.59	126.84	119.32
1	B	1906	ASP	C-N-CA	6.59	126.84	119.32
1	A	1730	CYS	N-CA-C	-6.46	98.32	108.14
1	A	1770	VAL	N-CA-C	6.44	117.22	110.72
1	B	2088	GLN	N-CA-C	-6.39	105.30	113.23
1	B	2012	MET	N-CA-C	6.35	120.41	110.32
1	A	1946	PRO	N-CA-C	-6.34	100.19	110.40
1	C	1966	GLU	N-CA-C	6.32	120.33	112.24
1	B	1946	PRO	N-CA-C	-6.30	101.75	111.13
1	A	1743	GLY	N-CA-C	-6.20	107.20	115.32
1	A	1990	PRO	CA-C-N	6.18	127.56	119.84
1	A	1990	PRO	C-N-CA	6.18	127.56	119.84
1	B	1533	THR	N-CA-C	-6.15	101.67	110.59
1	A	1685	GLU	N-CA-C	6.08	118.37	110.53
1	B	2112	GLU	N-CA-C	-6.04	99.85	109.76
1	B	1576	TYR	CA-C-N	6.01	127.35	119.84
1	B	1576	TYR	C-N-CA	6.01	127.35	119.84
1	B	1783	MET	N-CA-C	5.98	117.88	111.36
1	A	1733	VAL	N-CA-C	5.90	118.34	109.20
1	B	1879	VAL	N-CA-C	5.88	116.94	108.48
1	B	1743	GLY	N-CA-C	-5.86	107.64	115.32
1	B	1636	VAL	CB-CA-C	-5.82	108.18	114.35
1	A	1903	ILE	CA-C-N	5.80	125.71	119.85
1	A	1903	ILE	C-N-CA	5.80	125.71	119.85
1	C	1982	LYS	N-CA-C	5.75	120.29	112.88
1	B	1903	ILE	CA-C-N	5.71	125.68	120.03
1	B	1903	ILE	C-N-CA	5.71	125.68	120.03
1	C	1576	TYR	CA-C-N	5.69	125.36	119.05
1	C	1576	TYR	C-N-CA	5.69	125.36	119.05
1	C	2102	ARG	N-CA-C	-5.66	105.25	111.82
1	A	1909	ASN	CA-C-N	5.66	126.04	119.47
1	A	1909	ASN	C-N-CA	5.66	126.04	119.47
1	B	1556	GLU	CA-C-N	5.66	126.91	119.84
1	B	1556	GLU	C-N-CA	5.66	126.91	119.84
1	A	2192	GLU	N-CA-C	-5.62	105.11	112.41
1	B	1624	ASN	N-CA-C	5.50	117.15	108.96
1	C	1536	PHE	N-CA-C	-5.49	106.54	113.18
1	B	1939	PHE	N-CA-C	-5.47	105.34	112.23
1	C	1733	VAL	N-CA-C	5.45	117.65	109.20
1	B	1929	ALA	N-CA-C	-5.45	105.25	111.14
1	B	1677	THR	N-CA-C	5.40	117.62	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1556	GLU	CA-C-N	5.39	125.40	119.90
1	A	1556	GLU	C-N-CA	5.39	125.40	119.90
1	B	1638	LEU	N-CA-C	5.37	122.23	110.80
1	A	1624	ASN	N-CA-C	5.35	116.94	108.96
1	C	1572	LYS	N-CA-C	-5.34	100.46	108.96
1	C	1876	GLY	N-CA-C	-5.31	107.74	114.16
1	A	2087	GLY	N-CA-C	-5.24	106.37	113.24
1	A	1644	ASN	N-CA-C	-5.23	105.26	111.69
1	A	1785	ASN	N-CA-C	-5.20	106.45	112.89
1	A	1966	GLU	N-CA-C	5.19	118.88	112.24
1	B	1885	GLY	N-CA-C	-5.18	106.92	114.90
1	C	2004	ASP	CA-C-N	5.14	124.81	119.56
1	C	2004	ASP	C-N-CA	5.14	124.81	119.56
1	B	1966	GLU	N-CA-C	5.12	118.69	111.52
1	B	1571	VAL	CB-CA-C	-5.11	102.95	110.82
1	A	1675	VAL	N-CA-C	5.11	114.93	107.88
1	A	2112	GLU	N-CA-C	-5.10	101.39	109.76
1	A	1831	VAL	N-CA-C	-5.09	101.25	108.58
1	B	1909	ASN	CA-C-N	5.08	124.69	119.05
1	B	1909	ASN	C-N-CA	5.08	124.69	119.05
1	A	1568	LYS	N-CA-C	-5.04	101.03	109.24
1	A	1954	ARG	N-CA-C	-5.02	105.51	111.69
1	C	1850	ARG	N-CA-C	5.00	116.45	108.79
1	A	1657	TYR	N-CA-C	5.00	115.64	108.74
1	C	1783	MET	N-CA-C	5.00	118.64	112.54

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	5424	0	5365	226	0
1	B	5376	0	5316	251	0
1	C	5298	0	5234	234	0
2	A	34	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	34	0	28	2	0
2	C	34	0	28	1	0
All	All	16200	0	15999	682	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (682) 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:1936:ILE:HG12	1:A:1947:MET:HE1	1.43	1.01
1:A:1494:GLN:HA	1:A:1496:LYS:HE3	1.39	0.99
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.43	0.99
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.61	0.97
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.04	0.97
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.00	0.95
1:C:1638:LEU:H	1:C:1638:LEU:HD23	1.28	0.95
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.07	0.94
1:A:1824:LYS:HZ3	1:A:1824:LYS:H	1.12	0.93
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.17	0.92
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.12	0.91
1:B:2154:ARG:NH1	1:B:2158:TRP:HE1	1.69	0.91
1:A:1503:MET:HE3	1:A:1589:ILE:HG13	1.52	0.90
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.33	0.90
1:A:1683:ASN:ND2	1:A:1684:GLY:H	1.71	0.89
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.37	0.89
1:C:1781:GLN:H	1:C:1781:GLN:NE2	1.71	0.88
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.21	0.87
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.58	0.84
1:A:1494:GLN:CA	1:A:1496:LYS:HE3	2.06	0.84
1:A:1824:LYS:H	1:A:1824:LYS:NZ	1.77	0.83
1:A:1496:LYS:H	1:A:1496:LYS:HD3	1.43	0.83
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.76	0.82
1:C:1629:ILE:HD13	1:C:1629:ILE:H	1.45	0.82
1:C:1642:ALA:HB1	1:C:1644:ASN:HD22	1.46	0.81
1:A:1852:THR:HG22	1:A:1854:SER:H	1.45	0.80
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.64	0.80
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.17	0.79
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.80	0.79
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.64	0.78
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.30	0.78
1:B:2183:ASP:O	1:B:2187:LYS:HE3	1.84	0.78
1:B:2044:MET:SD	1:B:2082:LEU:HD21	2.24	0.77
1:C:1737:ALA:O	1:C:1740:VAL:HG13	1.85	0.77
1:B:1963:MET:HE3	1:C:1783:MET:HE1	1.65	0.76
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	1.99	0.75
1:C:2045:ASN:C	1:C:2045:ASN:HD22	1.94	0.75
1:B:2007:ILE:HB	1:B:2012:MET:HE1	1.68	0.75
1:C:1642:ALA:HB1	1:C:1644:ASN:ND2	2.02	0.75
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.79	0.75
1:C:1682:ILE:HG21	1:C:1687:ARG:CZ	2.17	0.75
1:C:2160:PRO:HG2	1:C:2163:VAL:HG23	1.68	0.75
1:B:1729:THR:O	1:B:1730:CYS:HB3	1.85	0.75
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.67	0.75
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.68	0.74
1:A:1524:LYS:HB2	1:A:1524:LYS:NZ	2.02	0.74
1:B:1852:THR:HG22	1:B:1855:GLY:O	1.88	0.74
1:B:1735:ILE:HD13	1:B:1735:ILE:O	1.88	0.74
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.87	0.73
1:C:2100:SER:O	1:C:2104:VAL:HG23	1.88	0.72
1:C:2129:ARG:NH1	1:C:2129:ARG:HB3	2.05	0.72
1:B:2154:ARG:HH11	1:B:2158:TRP:HE1	1.36	0.72
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.53	0.72
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.38	0.72
1:C:1773:SER:N	1:C:1776:GLN:HE21	1.85	0.72
1:B:1667:LYS:HG2	1:B:1672:GLU:HG2	1.72	0.71
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.87	0.71
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.38	0.71
1:B:1824:LYS:HG3	1:B:1825:ASP:H	1.54	0.71
1:C:2185:LYS:O	1:C:2189:LEU:HD13	1.91	0.71
1:B:1663:MET:HG3	1:B:1688:PHE:CD2	2.27	0.70
1:A:1939:PHE:HD1	1:A:1947:MET:HE3	1.55	0.70
1:A:2041:LEU:O	1:A:2044:MET:HB2	1.91	0.70
1:C:1493:LEU:HD12	1:C:1497:ARG:HH21	1.55	0.70
1:C:1911:ASN:HD22	1:C:1911:ASN:N	1.91	0.69
1:A:1533:THR:HB	1:A:1535:ASP:OD1	1.92	0.69
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.73	0.69
1:A:2189:LEU:O	1:A:2192:GLU:HB2	1.92	0.69
1:C:1824:LYS:HB2	1:C:1824:LYS:NZ	2.08	0.69
1:B:2000:TRP:CZ2	1:B:2014:MET:HE3	2.28	0.69
1:B:1564:MET:HE2	1:B:1604:PHE:HD1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1824:LYS:H	1:C:1824:LYS:HZ2	1.41	0.68
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.08	0.68
1:B:1612:ARG:HD3	1:B:1718:ALA:HA	1.75	0.68
1:C:1824:LYS:HB2	1:C:1824:LYS:HZ3	1.58	0.68
1:C:1796:ASP:O	1:C:1800:VAL:HG23	1.93	0.68
1:C:2104:VAL:HG22	1:C:2109:ILE:HD11	1.74	0.68
1:C:1638:LEU:HD23	1:C:1638:LEU:N	2.08	0.67
1:B:2110:SER:O	1:B:2111:LYS:HG3	1.93	0.67
1:A:1762:ILE:O	1:A:1766:LEU:HD13	1.95	0.67
1:C:1797:LEU:O	1:C:1801:GLU:HG3	1.94	0.67
1:B:1824:LYS:HG3	1:B:1825:ASP:N	2.08	0.67
1:B:2163:VAL:HA	1:B:2170:GLN:NE2	2.09	0.67
1:A:1683:ASN:HD22	1:A:1684:GLY:H	1.42	0.67
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.41	0.66
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.77	0.66
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.77	0.66
1:B:1775:LEU:O	1:B:1781:GLN:NE2	2.29	0.66
1:B:2046:ARG:HG2	1:C:1643:TRP:HH2	1.60	0.66
1:A:2143:VAL:HG22	1:A:2145:GLU:H	1.60	0.66
1:B:2146:ALA:O	1:B:2151:LYS:HE2	1.95	0.65
1:A:2041:LEU:HA	1:A:2044:MET:CG	2.26	0.65
1:A:1683:ASN:HD22	1:A:1684:GLY:N	1.94	0.65
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.44	0.65
1:A:1681:VAL:HG23	1:A:1685:GLU:O	1.96	0.65
1:C:1629:ILE:H	1:C:1629:ILE:CD1	2.08	0.65
1:C:1759:ALA:N	1:C:1774:ASN:HD21	1.89	0.65
1:B:2154:ARG:HH11	1:B:2158:TRP:NE1	1.95	0.65
1:B:2037:ARG:O	1:B:2041:LEU:HD13	1.97	0.64
1:B:1730:CYS:H	1:B:1752:GLN:HG3	1.62	0.64
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.79	0.64
1:A:1683:ASN:ND2	1:A:1684:GLY:N	2.45	0.64
1:B:1641:VAL:HG21	1:C:2089:ILE:HD13	1.80	0.64
1:C:1527:SER:O	1:C:1530:VAL:HG22	1.97	0.64
1:C:2045:ASN:C	1:C:2045:ASN:ND2	2.56	0.64
1:C:2148:ARG:HG3	1:C:2148:ARG:HH11	1.62	0.64
1:A:1939:PHE:CD1	1:A:1947:MET:HE3	2.33	0.64
1:A:1954:ARG:O	1:A:1996:ARG:HB2	1.97	0.64
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.95	0.63
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.63	0.63
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.32	0.63
1:A:1824:LYS:HZ3	1:A:1824:LYS:N	1.91	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2082:LEU:HD23	1:A:2082:LEU:H	1.62	0.63
1:B:2040:LEU:HD11	1:B:2086:TYR:O	1.98	0.62
1:A:1527:SER:O	1:A:1530:VAL:HG22	1.99	0.62
1:A:1633:GLU:O	1:A:1636:VAL:HG12	1.97	0.62
1:B:1677:THR:HG22	1:B:1690:ILE:HA	1.81	0.62
1:A:1903:ILE:N	1:A:1903:ILE:HD12	2.14	0.62
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.81	0.62
1:C:2041:LEU:O	1:C:2044:MET:HB2	1.99	0.62
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	1.79	0.62
1:A:1852:THR:HB	1:A:1855:GLY:O	1.99	0.62
1:C:2041:LEU:HA	1:C:2044:MET:HG3	1.81	0.62
1:C:2129:ARG:HB3	1:C:2129:ARG:CZ	2.28	0.62
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.64	0.62
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.29	0.62
1:C:1636:VAL:HB	1:C:1637:PRO:HD3	1.82	0.61
1:B:1643:TRP:CD1	1:B:1643:TRP:H	2.16	0.61
1:C:1644:ASN:HD21	1:C:1687:ARG:NH1	1.97	0.61
1:B:1786:ASN:OD1	1:C:1966:GLU:HG3	1.99	0.61
1:B:2085:ILE:HG13	1:C:1650:ASP:HA	1.82	0.61
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.83	0.61
1:B:1668:LYS:HD2	1:B:1669:PHE:CE2	2.36	0.61
1:B:1548:GLY:O	1:B:1606:LYS:HE2	2.00	0.61
1:C:2188:GLY:C	1:C:2189:LEU:HD12	2.25	0.61
1:C:1648:ASN:ND2	1:C:1651:LYS:HE2	2.16	0.61
1:A:1634:GLU:O	1:A:1634:GLU:HG2	2.01	0.61
1:C:1654:GLN:O	1:C:1655:TYR:HB3	2.00	0.61
1:A:1677:THR:CG2	1:A:1690:ILE:HG22	2.31	0.61
1:A:2190:LYS:C	1:A:2192:GLU:H	2.08	0.61
1:C:1681:VAL:HG22	1:C:1686:GLU:HA	1.82	0.61
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.65	0.60
1:A:1677:THR:HG22	1:A:1690:ILE:HG22	1.83	0.60
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.84	0.60
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.81	0.60
1:C:1638:LEU:H	1:C:1638:LEU:CD2	2.05	0.60
1:A:1944:GLN:HA	1:A:1983:GLN:NE2	2.17	0.60
1:C:1625:SER:HB3	1:C:1731:ARG:NH2	2.17	0.60
1:C:2148:ARG:HH12	1:C:2152:ILE:HD13	1.66	0.60
1:B:1657:TYR:CE2	1:B:1687:ARG:HG2	2.37	0.60
1:B:1966:GLU:HG2	1:C:1786:ASN:OD1	2.02	0.60
1:A:2143:VAL:HB	1:A:2192:GLU:OE1	2.02	0.59
1:A:1823:THR:HB	1:A:1824:LYS:HZ3	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.10	0.59
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.17	0.59
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.85	0.59
1:C:1794:VAL:HG23	1:C:1795:ASP:OD1	2.03	0.59
1:A:1852:THR:HG22	1:A:1853:GLU:N	2.16	0.59
1:A:1955:GLY:HA2	1:A:1999:SER:OG	2.02	0.58
1:B:2139:LEU:HD23	1:B:2151:LYS:HG2	1.85	0.58
1:B:1648:ASN:N	1:B:1649:PRO:HD3	2.18	0.58
1:B:2140:SER:O	1:B:2144:GLY:HA3	2.03	0.58
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.85	0.58
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	1.86	0.58
1:B:2031:VAL:HG13	1:B:2035:PHE:HB3	1.85	0.57
1:A:1682:ILE:C	1:A:1683:ASN:HD22	2.12	0.57
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	1.86	0.57
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.38	0.57
1:A:1524:LYS:HB2	1:A:1524:LYS:HZ2	1.69	0.57
1:B:2041:LEU:HA	1:B:2044:MET:HB2	1.86	0.57
1:C:1715:THR:HG22	1:C:1742:LEU:HB3	1.87	0.57
1:C:2041:LEU:HA	1:C:2044:MET:CG	2.34	0.57
1:A:1496:LYS:HD3	1:A:1496:LYS:N	2.15	0.57
1:A:1991:PRO:O	1:A:2019:ASN:O	2.22	0.57
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.87	0.57
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.12	0.57
1:C:2100:SER:HA	1:C:2103:MET:HE3	1.87	0.57
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.40	0.57
1:A:1877:VAL:HG23	1:A:1931:LYS:HD3	1.87	0.57
1:A:1901:ASN:HB3	1:A:1917:ILE:HB	1.87	0.56
1:C:1637:PRO:HB2	1:C:1638:LEU:HD23	1.85	0.56
1:A:1909:ASN:ND2	1:A:1911:ASN:H	2.03	0.56
1:C:2031:VAL:HG21	1:C:2091:LEU:HD23	1.87	0.56
1:A:1648:ASN:HB2	1:A:1651:LYS:HG2	1.85	0.56
1:B:2154:ARG:NH1	1:B:2158:TRP:NE1	2.47	0.56
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.13	0.56
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.38	0.56
1:C:1909:ASN:HD22	1:C:1912:SER:HB2	1.69	0.56
1:C:1629:ILE:HD13	1:C:1629:ILE:N	2.19	0.56
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.88	0.56
1:C:1781:GLN:HE21	1:C:1781:GLN:N	1.95	0.56
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.36	0.56
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.06	0.56
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1909:ASN:C	1:B:1909:ASN:HD22	2.14	0.55
1:B:1738:TYR:CE1	1:C:1968:LEU:HD12	2.41	0.55
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.88	0.55
1:C:1844:ARG:HH11	1:C:1844:ARG:HG3	1.72	0.55
1:B:2184:ASP:HA	1:B:2187:LYS:HB2	1.88	0.55
1:A:2158:TRP:CE2	1:A:2185:LYS:HD3	2.42	0.55
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.44	0.55
1:C:1782:ILE:O	1:C:1786:ASN:HB2	2.06	0.55
1:C:1911:ASN:N	1:C:1911:ASN:ND2	2.55	0.55
1:C:2187:LYS:C	1:C:2189:LEU:H	2.14	0.55
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.42	0.55
1:C:1568:LYS:HE2	1:C:1581:GLN:NE2	2.21	0.55
1:A:1725:ILE:HD12	1:A:1803:ILE:HG12	1.88	0.55
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.06	0.55
1:A:1936:ILE:CG1	1:A:1947:MET:HE1	2.27	0.54
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.07	0.54
1:A:2140:SER:OG	1:A:2151:LYS:HE3	2.07	0.54
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.73	0.54
1:B:1644:ASN:O	1:B:1645:ASP:HB2	2.07	0.54
1:A:2041:LEU:HA	1:A:2044:MET:HG2	1.89	0.54
1:B:2132:GLU:O	1:B:2136:ILE:HG13	2.07	0.54
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.90	0.54
1:C:2148:ARG:NH1	1:C:2152:ILE:HD13	2.22	0.54
1:A:1733:VAL:HG12	1:A:1734:GLY:N	2.21	0.54
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.88	0.54
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.07	0.54
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.88	0.54
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.21	0.54
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.71	0.54
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.05	0.54
1:B:1681:VAL:HG13	1:B:1685:GLU:O	2.06	0.54
1:C:1591:PHE:C	1:C:1591:PHE:CD2	2.86	0.54
1:C:1643:TRP:O	1:C:1645:ASP:N	2.40	0.54
1:A:2132:GLU:O	1:A:2136:ILE:HG13	2.08	0.54
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.05	0.54
1:C:1783:MET:SD	1:C:1786:ASN:ND2	2.80	0.54
1:A:1708:SER:OG	1:A:1735:ILE:HB	2.08	0.54
1:C:1530:VAL:O	1:C:1530:VAL:HG23	2.08	0.54
1:C:1851:GLU:OE1	1:C:1851:GLU:HA	2.08	0.54
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.90	0.54
1:B:1909:ASN:HD21	1:B:1911:ASN:CG	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.90	0.54
1:B:2044:MET:HA	1:B:2086:TYR:CE2	2.43	0.53
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.73	0.53
1:C:2044:MET:C	1:C:2046:ARG:H	2.16	0.53
1:A:1648:ASN:O	1:A:1651:LYS:HG2	2.09	0.53
1:A:1909:ASN:ND2	1:A:1909:ASN:C	2.66	0.53
1:B:1544:GLU:OE1	1:B:1602:GLU:OE1	2.25	0.53
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.27	0.53
1:A:1560:ASN:HD22	1:A:1560:ASN:N	2.06	0.53
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.91	0.53
1:B:1755:ILE:HD12	1:B:1758:GLY:HA2	1.90	0.53
1:C:1736:GLY:O	1:C:1740:VAL:HG12	2.09	0.53
1:B:1877:VAL:HG13	1:B:1931:LYS:HD3	1.90	0.52
1:B:2089:ILE:HD13	1:C:1653:PHE:CE2	2.43	0.52
1:C:2173:THR:O	1:C:2177:GLU:HB2	2.09	0.52
1:A:1753:PRO:HB3	1:A:1775:LEU:HD23	1.91	0.52
1:A:1766:LEU:N	1:A:1766:LEU:HD12	2.24	0.52
1:A:2043:THR:C	1:A:2045:ASN:H	2.15	0.52
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	1.91	0.52
1:B:1762:ILE:HD12	1:B:1777:LEU:HD21	1.91	0.52
1:B:2031:VAL:O	1:B:2033:ILE:N	2.42	0.52
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.44	0.52
1:C:1902:LEU:HD11	1:C:1914:GLU:OE2	2.09	0.52
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	1.90	0.52
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	1.91	0.52
1:C:1679:ARG:NH2	1:C:1686:GLU:HG2	2.24	0.52
1:C:2083:LEU:HB2	1:C:2084:PRO:HD3	1.89	0.52
1:B:2008:ASN:H	1:B:2012:MET:HE3	1.75	0.52
1:A:2187:LYS:O	1:A:2190:LYS:HG2	2.10	0.52
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.09	0.52
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.58	0.52
1:A:1682:ILE:O	1:A:1683:ASN:C	2.53	0.52
1:B:1730:CYS:H	1:B:1752:GLN:CG	2.23	0.52
1:B:1809:TYR:O	1:B:1945:LEU:HD21	2.10	0.52
1:B:2046:ARG:HG2	1:C:1643:TRP:CH2	2.44	0.52
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.07	0.52
1:B:1852:THR:HG23	1:B:1854:SER:H	1.75	0.52
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.40	0.52
1:C:1657:TYR:CD2	1:C:1687:ARG:HG3	2.44	0.52
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.45	0.51
1:A:1648:ASN:HB2	1:A:1651:LYS:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.91	0.51
1:A:1634:GLU:OE2	1:A:1634:GLU:N	2.40	0.51
1:C:2142:GLN:HG3	1:C:2142:GLN:O	2.11	0.51
1:A:2140:SER:C	1:A:2142:GLN:H	2.18	0.51
1:B:2046:ARG:HB3	1:B:2086:TYR:OH	2.11	0.51
1:A:1766:LEU:N	1:A:1766:LEU:CD1	2.73	0.51
1:B:2035:PHE:CD1	1:C:1631:MET:HE1	2.46	0.51
1:B:1958:GLY:H	2:B:1:B36:CAM	2.23	0.51
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.10	0.51
1:B:1909:ASN:C	1:B:1909:ASN:ND2	2.68	0.51
1:C:2090:SER:O	1:C:2093:PHE:HB3	2.11	0.51
1:B:1576:TYR:N	1:B:1577:PRO:HD3	2.26	0.51
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.10	0.51
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.45	0.51
1:B:1708:SER:CB	1:B:1735:ILE:HG13	2.41	0.51
1:B:1975:VAL:O	1:B:1979:VAL:HG23	2.11	0.51
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.46	0.51
1:A:1605:ASN:O	1:A:1609:GLU:HG3	2.10	0.51
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.10	0.51
1:C:1955:GLY:HA2	1:C:1999:SER:HB3	1.93	0.51
1:C:1682:ILE:HG23	1:C:1682:ILE:O	2.11	0.51
1:B:1782:ILE:CG2	1:B:1783:MET:HE2	2.41	0.50
1:C:1643:TRP:O	1:C:1644:ASN:C	2.55	0.50
1:A:1981:TYR:CD2	1:A:1985:ILE:HD11	2.45	0.50
1:A:2008:ASN:C	1:A:2008:ASN:ND2	2.69	0.50
1:B:1649:PRO:C	1:B:1651:LYS:H	2.18	0.50
1:B:1757:THR:HG22	1:B:1762:ILE:HG13	1.93	0.50
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.19	0.50
1:B:1582:PHE:CD2	1:B:1807:MET:HE1	2.46	0.50
1:A:1852:THR:CG2	1:A:1853:GLU:N	2.74	0.50
1:B:1650:ASP:HA	1:C:2085:ILE:HB	1.94	0.50
1:C:1998:GLY:O	1:C:2001:VAL:HG22	2.12	0.50
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	1.93	0.50
1:C:1680:THR:O	1:C:1687:ARG:HB3	2.11	0.50
1:A:1608:THR:O	1:A:1612:ARG:HG2	2.12	0.50
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.12	0.50
1:B:1556:GLU:HG3	1:B:1559:ALA:HB2	1.94	0.50
1:B:1729:THR:O	1:B:1730:CYS:CB	2.56	0.50
1:B:1776:GLN:O	1:C:1960:GLN:HG3	2.12	0.50
1:B:1782:ILE:HG22	1:B:1783:MET:HE2	1.93	0.50
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1682:ILE:O	1:C:1683:ASN:C	2.54	0.50
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.49	0.50
1:C:2146:ALA:O	1:C:2151:LYS:HE3	2.12	0.50
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.89	0.50
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.94	0.50
1:A:2041:LEU:HA	1:A:2044:MET:HG3	1.93	0.49
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.59	0.49
1:C:2096:LEU:HD23	1:C:2099:ARG:NH2	2.27	0.49
1:C:1733:VAL:HG12	1:C:1734:GLY:N	2.25	0.49
1:C:2000:TRP:CD1	1:C:2000:TRP:C	2.90	0.49
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.94	0.49
1:C:2008:ASN:HB3	1:C:2012:MET:HG3	1.93	0.49
1:A:1612:ARG:CD	1:A:1718:ALA:HA	2.42	0.49
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.75	0.49
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.12	0.49
1:A:2081:GLU:CD	1:A:2081:GLU:N	2.70	0.49
1:B:1861:PHE:CE2	1:B:1889:LEU:HD21	2.48	0.49
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.94	0.49
1:C:1873:TRP:O	1:C:1874:ALA:C	2.54	0.49
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.27	0.49
1:A:1909:ASN:C	1:A:1909:ASN:HD22	2.20	0.49
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.21	0.49
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.12	0.49
1:A:1649:PRO:C	1:A:1651:LYS:H	2.21	0.49
1:A:2149:LEU:HD12	1:A:2149:LEU:O	2.13	0.49
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.94	0.49
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.76	0.49
1:C:1852:THR:HG22	1:C:1854:SER:H	1.78	0.49
1:A:2190:LYS:C	1:A:2192:GLU:N	2.69	0.49
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.12	0.49
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.43	0.49
1:A:1564:MET:HE3	1:A:1604:PHE:HB2	1.95	0.49
1:A:2031:VAL:HG23	1:A:2032:GLY:N	2.28	0.49
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.94	0.49
1:C:1591:PHE:C	1:C:1591:PHE:HD2	2.20	0.49
1:A:1496:LYS:HZ3	1:A:1558:GLY:HA3	1.78	0.49
1:B:2148:ARG:HG3	1:B:2148:ARG:HH11	1.78	0.49
1:B:1543:ILE:CD1	1:B:1553:VAL:HG11	2.43	0.48
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.13	0.48
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	1.95	0.48
1:B:2096:LEU:HD23	1:B:2099:ARG:NH2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1505:THR:HB	1:C:1730:CYS:HB2	1.94	0.48
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.47	0.48
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.38	0.48
1:B:2110:SER:O	1:B:2111:LYS:CG	2.61	0.48
1:B:2148:ARG:HG3	1:B:2148:ARG:NH1	2.28	0.48
1:C:1759:ALA:N	1:C:1760:PRO:HD2	2.28	0.48
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.21	0.48
1:A:1958:GLY:H	2:A:1:B36:CAM	2.27	0.48
1:A:2022:ALA:HB3	1:A:2103:MET:HE2	1.95	0.48
1:C:1902:LEU:C	1:C:1902:LEU:HD13	2.38	0.48
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.61	0.48
1:B:2152:ILE:O	1:B:2156:ARG:HG2	2.13	0.48
1:C:1644:ASN:HD21	1:C:1687:ARG:HH12	1.60	0.48
1:B:1576:TYR:CE2	1:B:1812:ALA:HB2	2.49	0.48
1:B:1644:ASN:HD21	1:B:1654:GLN:HE21	1.60	0.48
1:C:1619:ILE:HD13	1:C:1619:ILE:N	2.29	0.48
1:C:2036:ARG:HB3	1:C:2036:ARG:NH1	2.28	0.48
1:B:1576:TYR:CZ	1:B:1812:ALA:HB2	2.49	0.48
1:B:1733:VAL:HG12	1:B:1734:GLY:N	2.28	0.48
1:B:1827:TRP:HA	1:B:2119:ARG:NH1	2.29	0.48
1:C:1677:THR:HA	1:C:1689:VAL:O	2.13	0.48
1:C:1786:ASN:HB3	1:C:1788:VAL:H	1.79	0.48
1:B:2000:TRP:CH2	1:B:2014:MET:HE3	2.49	0.48
1:B:1754:ILE:O	1:B:1778:GLY:HA3	2.13	0.48
1:B:2104:VAL:HG21	1:B:2112:GLU:HG2	1.96	0.48
1:A:1524:LYS:HB2	1:A:1524:LYS:HZ3	1.79	0.48
1:B:1653:PHE:CD1	1:B:1653:PHE:N	2.82	0.48
1:C:1697:GLU:O	1:C:1700:LEU:HD13	2.14	0.48
1:C:1991:PRO:C	1:C:1992:THR:HG23	2.39	0.48
1:A:1795:ASP:O	1:A:1798:ALA:HB3	2.14	0.47
1:B:1768:ARG:CB	1:B:1768:ARG:HH11	2.26	0.47
1:C:2045:ASN:ND2	1:C:2045:ASN:O	2.47	0.47
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.63	0.47
1:B:1575:GLU:C	1:B:1577:PRO:HD3	2.39	0.47
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.44	0.47
1:B:2147:SER:HB3	1:B:2150:GLU:OE2	2.14	0.47
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.14	0.47
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.29	0.47
1:C:1619:ILE:HD12	1:C:1725:ILE:HG22	1.96	0.47
1:C:2125:ARG:O	1:C:2129:ARG:HG2	2.14	0.47
1:A:1575:GLU:HB3	1:A:1819:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2043:THR:C	1:A:2045:ASN:N	2.72	0.47
1:B:2047:LEU:HD13	1:B:2047:LEU:C	2.40	0.47
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.79	0.47
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.63	0.47
1:B:1836:THR:HG22	1:B:1838:ASP:OD2	2.14	0.47
1:B:1996:ARG:NE	1:B:2026:GLU:HG2	2.30	0.47
1:B:1996:ARG:O	1:B:1997:GLY:C	2.57	0.47
1:C:2187:LYS:C	1:C:2189:LEU:N	2.73	0.47
1:A:1668:LYS:O	1:A:1668:LYS:HG2	2.14	0.47
1:A:1781:GLN:CD	1:A:1781:GLN:H	2.21	0.47
1:A:2045:ASN:O	1:A:2046:ARG:HD2	2.15	0.47
1:B:1960:GLN:HE21	1:B:1960:GLN:C	2.21	0.47
1:C:1909:ASN:ND2	1:C:1912:SER:HB2	2.30	0.47
1:A:1659:THR:OG1	1:A:1661:GLU:HB3	2.14	0.47
1:B:2156:ARG:HG3	1:B:2156:ARG:NH1	2.28	0.47
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.39	0.47
1:C:1755:ILE:HD12	1:C:1758:GLY:HA2	1.95	0.47
1:C:1785:ASN:HA	1:C:1872:GLY:O	2.15	0.47
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.29	0.47
1:A:1730:CYS:O	1:A:1731:ARG:C	2.56	0.47
1:A:1748:GLN:O	1:A:1792:THR:HA	2.15	0.47
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.61	0.47
1:C:1493:LEU:CD1	1:C:1497:ARG:HH21	2.25	0.47
1:C:2005:PRO:HG3	1:C:2014:MET:HB2	1.96	0.47
1:A:2096:LEU:HA	1:A:2099:ARG:NH1	2.30	0.46
1:B:2096:LEU:HD23	1:B:2099:ARG:CZ	2.46	0.46
1:C:1639:PHE:CD1	1:C:1639:PHE:C	2.94	0.46
1:C:2085:ILE:O	1:C:2089:ILE:HG13	2.15	0.46
1:C:2148:ARG:HH11	1:C:2148:ARG:CG	2.27	0.46
1:B:1603:PHE:O	1:B:1607:VAL:HG23	2.15	0.46
1:C:1666:LEU:HD22	1:C:1671:LYS:O	2.15	0.46
1:C:1766:LEU:O	1:C:1768:ARG:N	2.46	0.46
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.48	0.46
1:C:2139:LEU:HD21	1:C:2154:ARG:HD2	1.97	0.46
1:A:1619:ILE:HD12	1:A:1619:ILE:N	2.29	0.46
1:A:1754:ILE:O	1:A:1778:GLY:HA3	2.14	0.46
1:B:1592:LYS:O	1:B:1593:ILE:HG12	2.16	0.46
1:B:1655:TYR:C	1:B:1656:LEU:HD12	2.40	0.46
1:B:1909:ASN:ND2	1:B:1911:ASN:H	2.13	0.46
1:C:1592:LYS:C	1:C:1593:ILE:HG12	2.40	0.46
1:C:1766:LEU:HD13	1:C:1770:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.13	0.46
1:C:1605:ASN:HD22	1:C:1714:ALA:HB2	1.81	0.46
1:B:2046:ARG:NH1	1:C:1639:PHE:O	2.48	0.46
1:C:1654:GLN:O	1:C:1655:TYR:CB	2.63	0.46
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.46	0.46
1:A:1982:LYS:HB2	1:A:1983:GLN:OE1	2.16	0.46
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	1.98	0.46
1:A:2138:ARG:HB3	1:A:2186:LEU:HD13	1.97	0.46
1:C:1650:ASP:C	1:C:1652:GLY:H	2.23	0.46
1:A:1823:THR:HB	1:A:1824:LYS:NZ	2.31	0.46
1:B:1629:ILE:HD13	1:C:2025:LEU:HD11	1.98	0.46
1:B:1682:ILE:CG1	1:B:1687:ARG:HD2	2.46	0.46
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.98	0.46
1:A:1619:ILE:HG13	1:A:1725:ILE:HG22	1.97	0.45
1:A:1765:MET:C	1:A:1767:GLY:H	2.24	0.45
1:A:2135:LEU:HD23	1:A:2155:ILE:CG2	2.46	0.45
1:B:1649:PRO:O	1:B:1651:LYS:N	2.46	0.45
1:B:2020:ALA:O	1:B:2021:ARG:HD2	2.16	0.45
1:C:1899:VAL:HB	1:C:1919:GLU:HB2	1.99	0.45
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.80	0.45
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.16	0.45
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.48	0.45
1:A:1496:LYS:H	1:A:1496:LYS:CD	2.07	0.45
1:A:1766:LEU:CD1	1:A:1766:LEU:H	2.29	0.45
1:A:1906:ASP:H	1:A:1912:SER:HG	1.63	0.45
1:B:1640:GLN:OE1	1:B:1659:THR:HG23	2.16	0.45
1:B:1829:ARG:HG3	1:B:1829:ARG:HH11	1.82	0.45
1:B:1909:ASN:HD22	1:B:1910:PRO:N	2.15	0.45
1:B:2101:SER:HB2	1:C:1692:THR:HG21	1.98	0.45
1:C:1592:LYS:O	1:C:1593:ILE:CG1	2.65	0.45
1:C:1844:ARG:HG3	1:C:1844:ARG:NH1	2.28	0.45
1:A:1630:GLY:C	1:A:1700:LEU:HD22	2.41	0.45
1:A:1644:ASN:ND2	1:A:1652:GLY:C	2.75	0.45
1:A:1649:PRO:O	1:A:1651:LYS:N	2.49	0.45
1:A:2135:LEU:HD23	1:A:2155:ILE:HG23	1.97	0.45
1:B:1838:ASP:O	1:B:1839:GLU:HB2	2.15	0.45
1:C:2025:LEU:HD22	2:C:1:B36:HAK	1.98	0.45
1:B:2035:PHE:HD2	1:B:2090:SER:CB	2.30	0.45
1:A:2000:TRP:CD1	1:A:2000:TRP:O	2.69	0.45
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.52	0.45
1:B:1972:SER:HB3	1:C:1742:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2100:SER:O	1:B:2104:VAL:HG23	2.17	0.45
1:C:1783:MET:HG3	1:C:1788:VAL:HB	1.98	0.45
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	1.99	0.45
1:A:2190:LYS:O	1:A:2192:GLU:N	2.41	0.45
1:B:1510:ASP:O	1:B:1513:GLU:HB3	2.15	0.45
1:B:1708:SER:HB3	1:B:1735:ILE:HG13	1.99	0.45
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.98	0.45
1:B:1997:GLY:HA2	1:C:1705:LEU:CD2	2.47	0.45
1:B:2008:ASN:N	1:B:2012:MET:HE3	2.31	0.45
1:C:2097:HIS:O	1:C:2102:ARG:HD3	2.17	0.45
1:A:1655:TYR:CE1	1:A:1689:VAL:HG22	2.52	0.45
1:B:2013:GLU:OE1	1:B:2125:ARG:NH2	2.38	0.45
1:A:1727:LEU:HD12	1:A:1747:ILE:O	2.17	0.44
1:A:1835:PRO:HG2	1:A:1991:PRO:HB2	1.99	0.44
1:B:2133:GLU:OE1	1:B:2148:ARG:NH2	2.49	0.44
1:C:1587:ASN:HB2	1:C:1623:ALA:O	2.17	0.44
1:B:1629:ILE:CD1	1:C:2025:LEU:HD11	2.46	0.44
1:B:1952:ASN:HA	1:B:1994:GLU:O	2.17	0.44
1:C:1608:THR:O	1:C:1612:ARG:HG3	2.16	0.44
1:A:1508:VAL:HG13	1:A:1509:TYR:N	2.32	0.44
1:A:1787:GLY:HA3	1:A:1873:TRP:CE3	2.52	0.44
1:A:2094:ALA:O	1:A:2097:HIS:HB2	2.17	0.44
1:A:2162:SER:HB3	1:B:1797:LEU:HB3	2.00	0.44
1:B:1856:PHE:CZ	1:B:1863:LYS:HG3	2.52	0.44
1:B:2106:LYS:HE2	1:B:2106:LYS:HA	1.99	0.44
1:A:1733:VAL:O	1:A:1736:GLY:N	2.48	0.44
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.48	0.44
1:A:2031:VAL:C	1:A:2033:ILE:N	2.76	0.44
1:C:1909:ASN:HA	1:C:1910:PRO:HD3	1.79	0.44
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	1.99	0.44
1:A:1605:ASN:HD22	1:A:1714:ALA:CB	2.30	0.44
1:A:1756:LEU:HD12	1:A:1756:LEU:HA	1.77	0.44
1:A:2037:ARG:HG3	1:A:2037:ARG:HH11	1.83	0.44
1:B:1955:GLY:HA2	1:B:1999:SER:HB3	1.98	0.44
1:B:1836:THR:HB	1:B:1839:GLU:HB3	2.00	0.44
1:B:1991:PRO:O	1:B:1992:THR:OG1	2.35	0.44
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	1.98	0.44
1:A:2031:VAL:C	1:A:2033:ILE:H	2.26	0.43
1:B:1663:MET:O	1:B:1667:LYS:HG3	2.18	0.43
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.82	0.43
1:B:1841:TYR:CZ	1:B:1896:THR:HG21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	2.00	0.43
1:C:1648:ASN:HD21	1:C:1651:LYS:HE2	1.82	0.43
1:C:1781:GLN:NE2	1:C:1781:GLN:N	2.51	0.43
1:A:1662:GLY:C	1:A:1664:GLU:N	2.76	0.43
1:A:2143:VAL:HG22	1:A:2145:GLU:N	2.30	0.43
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.19	0.43
1:B:1925:HIS:O	1:B:1926:PRO:C	2.54	0.43
1:B:2035:PHE:CD1	1:B:2039:LYS:HD2	2.54	0.43
1:C:1682:ILE:HD13	1:C:1687:ARG:NH1	2.33	0.43
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.18	0.43
1:C:2128:ARG:HD3	1:C:2128:ARG:C	2.43	0.43
1:A:1614:ARG:HG3	1:A:1614:ARG:NH1	2.33	0.43
1:B:1873:TRP:O	1:B:1874:ALA:C	2.61	0.43
1:B:2000:TRP:CD1	1:B:2000:TRP:C	2.95	0.43
1:C:1715:THR:CG2	1:C:1742:LEU:HB3	2.48	0.43
1:C:2085:ILE:HG23	1:C:2086:TYR:HD1	1.83	0.43
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.83	0.43
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.82	0.43
1:C:1633:GLU:HA	1:C:1636:VAL:HG23	2.00	0.43
1:C:1619:ILE:HD12	1:C:1725:ILE:CG2	2.49	0.43
1:A:1636:VAL:CG1	1:A:1637:PRO:HD3	2.48	0.43
1:A:1649:PRO:C	1:A:1651:LYS:N	2.77	0.43
1:B:1981:TYR:CB	1:B:1985:ILE:HD11	2.48	0.43
1:C:1668:LYS:C	1:C:1670:ASP:H	2.27	0.43
1:A:1827:TRP:CZ3	1:A:2120:ARG:HG2	2.54	0.43
1:A:2172:ALA:O	1:A:2176:GLU:HG3	2.19	0.43
1:B:1862:ASP:OD1	1:B:2119:ARG:NH2	2.52	0.43
1:B:1995:LEU:HD12	1:B:1995:LEU:HA	1.89	0.43
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.54	0.43
1:C:2160:PRO:HG2	1:C:2163:VAL:CG2	2.44	0.43
1:A:1991:PRO:C	1:A:1993:GLY:H	2.27	0.43
1:C:1508:VAL:CG2	1:C:1588:ASP:HA	2.48	0.43
1:C:1798:ALA:O	1:C:1802:LYS:HG2	2.18	0.43
1:B:1533:THR:HB	1:B:1535:ASP:OD2	2.19	0.43
1:C:1646:ALA:HB1	1:C:1648:ASN:OD1	2.19	0.43
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.18	0.43
1:A:1743:GLY:O	1:A:1744:GLN:HB2	2.18	0.42
1:A:1902:LEU:HD13	1:A:1916:LEU:HD13	2.00	0.42
1:A:2021:ARG:HD2	1:A:2098:ASP:HB2	2.01	0.42
1:B:1514:LEU:HD22	1:B:1797:LEU:HG	2.00	0.42
1:B:1662:GLY:C	1:B:1664:GLU:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1735:ILE:O	1:B:1739:LEU:HG	2.17	0.42
1:C:1585:VAL:CG2	1:C:1607:VAL:HG11	2.49	0.42
1:B:1619:ILE:N	1:B:1619:ILE:HD12	2.33	0.42
1:C:1545:ASP:OD1	1:C:1547:ASN:N	2.45	0.42
1:C:1936:ILE:CG2	1:C:1977:ALA:HB1	2.49	0.42
1:C:1996:ARG:O	1:C:1997:GLY:C	2.61	0.42
1:C:2154:ARG:HG3	1:C:2154:ARG:NH1	2.34	0.42
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.49	0.42
1:A:1873:TRP:O	1:A:1874:ALA:C	2.62	0.42
1:C:1511:PHE:HA	1:C:1514:LEU:HD22	2.00	0.42
1:C:1643:TRP:HA	1:C:1653:PHE:HA	2.00	0.42
1:C:1648:ASN:HA	1:C:1649:PRO:HD3	1.78	0.42
1:C:1846:MET:HE1	1:C:1990:PRO:HB2	2.01	0.42
1:A:1638:LEU:HD12	1:A:1638:LEU:C	2.45	0.42
1:A:2148:ARG:HE	1:A:2148:ARG:HB2	1.67	0.42
1:B:1624:ASN:HD22	1:B:1626:GLY:N	2.17	0.42
1:B:1663:MET:HE2	1:B:1688:PHE:CD1	2.54	0.42
1:B:1701:GLY:O	1:B:1704:CYS:HB2	2.20	0.42
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.54	0.42
1:C:1503:MET:HB2	1:C:1505:THR:HG22	2.01	0.42
1:C:1635:ILE:HG22	1:C:1635:ILE:O	2.19	0.42
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.20	0.42
1:A:2008:ASN:HD21	1:A:2010:ASP:HB2	1.84	0.42
1:A:2082:LEU:H	1:A:2082:LEU:CD2	2.31	0.42
1:B:1852:THR:HG23	1:B:1854:SER:N	2.35	0.42
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.79	0.42
1:B:1682:ILE:O	1:B:1683:ASN:C	2.63	0.42
1:A:1606:LYS:HD2	1:A:1606:LYS:HA	1.83	0.42
1:A:1669:PHE:O	1:A:1671:LYS:HG3	2.20	0.42
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.53	0.42
1:B:1820:ILE:HG22	1:B:1821:LEU:N	2.35	0.42
1:B:2139:LEU:CD2	1:B:2151:LYS:HG2	2.50	0.42
1:A:1832:ASP:O	1:A:1833:PHE:C	2.63	0.42
1:B:1739:LEU:HD23	1:B:1739:LEU:HA	1.79	0.42
1:C:1824:LYS:NZ	1:C:1824:LYS:CB	2.80	0.42
1:A:1769:GLU:HG3	1:A:1769:GLU:O	2.20	0.42
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	2.01	0.42
1:B:1586:ALA:CB	1:B:1621:LEU:HB2	2.50	0.42
1:B:1705:LEU:HA	1:B:1705:LEU:HD23	1.78	0.42
1:B:2100:SER:HA	1:B:2103:MET:HE3	2.01	0.42
1:B:2183:ASP:O	1:B:2187:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1927:ASN:OD1	1:C:1928:SER:N	2.53	0.42
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.92	0.42
1:A:1782:ILE:O	1:A:1786:ASN:HB2	2.19	0.42
1:A:1952:ASN:HA	1:A:1994:GLU:O	2.20	0.42
1:B:1494:GLN:OE1	1:B:1496:LYS:HB2	2.20	0.42
1:B:1522:GLN:OE1	1:B:1804:VAL:HG13	2.20	0.42
1:B:2031:VAL:C	1:B:2033:ILE:H	2.28	0.42
1:C:1664:GLU:O	1:C:1665:THR:C	2.63	0.42
1:B:2147:SER:HB3	1:B:2150:GLU:CD	2.45	0.41
1:B:2142:GLN:HB3	1:B:2143:VAL:H	1.57	0.41
1:C:1575:GLU:CD	1:C:1575:GLU:N	2.77	0.41
1:C:1762:ILE:HA	1:C:1765:MET:HE2	2.02	0.41
1:C:1995:LEU:HD12	1:C:1995:LEU:HA	1.90	0.41
1:A:1516:ARG:HA	1:A:1537:PHE:CD2	2.55	0.41
1:A:1699:GLY:HA2	1:A:1704:CYS:SG	2.61	0.41
1:A:1691:LYS:HA	1:A:1691:LYS:HD3	1.88	0.41
1:A:1996:ARG:O	1:A:1997:GLY:C	2.63	0.41
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.20	0.41
1:B:1842:ASP:O	1:B:1843:VAL:C	2.64	0.41
1:A:1697:GLU:OE2	1:A:1697:GLU:HA	2.19	0.41
1:A:1733:VAL:CG1	1:A:1734:GLY:N	2.82	0.41
1:A:2178:ASN:O	1:A:2179:TYR:C	2.63	0.41
1:C:1894:VAL:HG22	1:C:1953:TRP:CZ2	2.55	0.41
1:B:1823:THR:O	1:B:1824:LYS:C	2.62	0.41
1:B:1965:ASN:C	1:B:1966:GLU:HG3	2.46	0.41
1:C:1562:ILE:HB	1:C:1600:GLU:OE2	2.21	0.41
1:C:1592:LYS:O	1:C:1593:ILE:HG12	2.21	0.41
1:C:1610:TYR:CE1	1:C:1614:ARG:CZ	3.04	0.41
1:C:1701:GLY:O	1:C:1704:CYS:HB2	2.21	0.41
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.56	0.41
1:A:1903:ILE:N	1:A:1903:ILE:CD1	2.81	0.41
1:B:1655:TYR:O	1:B:1656:LEU:HD12	2.21	0.41
1:B:2031:VAL:C	1:B:2033:ILE:N	2.79	0.41
2:B:1:B36:HARA	1:C:1765:MET:SD	2.60	0.41
1:C:1691:LYS:HA	1:C:1691:LYS:HE2	2.01	0.41
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.21	0.41
1:A:2177:GLU:O	1:B:1501:HIS:HE1	2.03	0.41
1:B:1783:MET:CE	1:C:1963:MET:HE3	2.50	0.41
1:B:1988:TYR:HA	1:B:2015:TYR:O	2.21	0.41
1:C:1514:LEU:HD12	1:C:1514:LEU:HA	1.88	0.41
1:C:1640:GLN:HG3	1:C:1659:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1645:ASP:O	1:C:1646:ALA:HB2	2.21	0.41
1:C:1991:PRO:O	1:C:1992:THR:HG23	2.20	0.41
1:A:1585:VAL:HG22	1:A:1607:VAL:HG11	2.03	0.41
1:A:1911:ASN:O	1:A:1912:SER:C	2.64	0.41
1:B:1533:THR:HG22	1:B:1534:ASP:N	2.35	0.41
1:B:1556:GLU:CG	1:B:1559:ALA:HB2	2.50	0.41
1:B:1824:LYS:HB2	1:B:1824:LYS:NZ	2.36	0.41
1:B:2028:GLN:CD	1:B:2028:GLN:H	2.29	0.41
1:C:1705:LEU:O	1:C:1708:SER:HB2	2.21	0.41
1:C:1988:TYR:HA	1:C:2015:TYR:O	2.21	0.41
1:B:1730:CYS:O	1:B:1731:ARG:O	2.38	0.41
1:B:2149:LEU:HD13	1:B:2149:LEU:O	2.20	0.41
1:C:1784:TYR:CE2	1:C:1872:GLY:HA3	2.56	0.41
1:B:2022:ALA:HB3	1:B:2103:MET:HE2	2.02	0.40
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.21	0.40
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.69	0.40
1:A:1545:ASP:OD2	1:A:1545:ASP:C	2.65	0.40
1:A:1634:GLU:O	1:A:1634:GLU:CG	2.70	0.40
1:B:1576:TYR:CE1	1:B:1819:PRO:HB3	2.57	0.40
1:B:2128:ARG:HE	1:B:2132:GLU:CD	2.30	0.40
1:C:1520:SER:O	1:C:1524:LYS:HG2	2.20	0.40
1:C:1648:ASN:ND2	1:C:1651:LYS:HG2	2.37	0.40
1:C:1730:CYS:O	1:C:1731:ARG:C	2.64	0.40
1:C:2036:ARG:HB3	1:C:2036:ARG:HH11	1.86	0.40
1:A:1719:TYR:O	1:A:1719:TYR:CG	2.73	0.40
1:A:1925:HIS:O	1:A:1926:PRO:C	2.62	0.40
1:A:2021:ARG:HH11	1:A:2021:ARG:HG2	1.86	0.40
1:B:1511:PHE:CD1	1:B:1621:LEU:HD13	2.57	0.40
1:B:1733:VAL:O	1:B:1736:GLY:N	2.50	0.40
1:B:1894:VAL:HG22	1:B:1953:TRP:CE2	2.57	0.40
1:A:1560:ASN:N	1:A:1560:ASN:ND2	2.70	0.40
1:B:1648:ASN:N	1:B:1649:PRO:CD	2.83	0.40
1:C:1582:PHE:CD2	1:C:1807:MET:HE1	2.55	0.40
1:C:1644:ASN:ND2	1:C:1687:ARG:HH12	2.19	0.40
1:A:2114:GLU:O	1:A:2115:TRP:C	2.63	0.40
1:B:2004:ASP:OD2	1:B:2006:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	677/769 (88%)	608 (90%)	58 (9%)	11 (2%)	7	27
1	B	671/769 (87%)	589 (88%)	63 (9%)	19 (3%)	4	14
1	C	661/769 (86%)	585 (88%)	60 (9%)	16 (2%)	4	17
All	All	2009/2307 (87%)	1782 (89%)	181 (9%)	46 (2%)	5	18

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	B	1643	TRP
1	B	1731	ARG
1	B	1839	GLU
1	B	2142	GLN
1	B	2145	GLU
1	C	1644	ASN
1	C	1655	TYR
1	A	1650	ASP
1	A	1684	GLY
1	A	1997	GLY
1	B	1645	ASP
1	B	1650	ASP
1	B	1766	LEU
1	B	1997	GLY
1	B	2032	GLY
1	C	1650	ASP
1	C	1768	ARG
1	C	1997	GLY
1	C	2037	ARG
1	A	1731	ARG
1	A	1991	PRO
1	A	2141	HIS
1	B	1683	ASN

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Mol	Chain	Res	Type
1	B	2046	ARG
1	C	1632	ALA
1	C	2145	GLU
1	A	1912	SER
1	A	2036	ARG
1	B	1824	LYS
1	B	2147	SER
1	C	1683	ASN
1	C	1744	GLN
1	C	2144	GLY
1	B	1655	TYR
1	B	1730	CYS
1	A	1635	ILE
1	B	1557	PRO
1	C	1508	VAL
1	C	1637	PRO
1	C	1649	PRO
1	B	1558	GLY
1	C	2084	PRO
1	A	1702	VAL
1	B	1637	PRO
1	C	1593	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/658 (88%)	541 (94%)	36 (6%)	16	45
1	B	572/658 (87%)	530 (93%)	42 (7%)	13	38
1	C	563/658 (86%)	524 (93%)	39 (7%)	14	41
All	All	1712/1974 (87%)	1595 (93%)	117 (7%)	14	42

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1496	LYS
1	A	1503	MET
1	A	1524	LYS
1	A	1532	LEU
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1640	GLN
1	A	1641	VAL
1	A	1651	LYS
1	A	1676	LEU
1	A	1681	VAL
1	A	1683	ASN
1	A	1708	SER
1	A	1725	ILE
1	A	1756	LEU
1	A	1766	LEU
1	A	1773	SER
1	A	1781	GLN
1	A	1786	ASN
1	A	1824	LYS
1	A	1837	ASN
1	A	1871	SER
1	A	1879	VAL
1	A	1884	LEU
1	A	1903	ILE
1	A	1924	TRP
1	A	1947	MET
1	A	1950	LEU
1	A	1991	PRO
1	A	2081	GLU
1	A	2084	PRO
1	A	2091	LEU
1	A	2135	LEU
1	A	2185	LYS
1	B	1485	THR
1	B	1490	LYS
1	B	1493	LEU
1	B	1494	GLN
1	B	1502	LEU
1	B	1508	VAL
1	B	1568	LYS

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Mol	Chain	Res	Type
1	B	1571	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1613	LYS
1	B	1616	ILE
1	B	1618	ARG
1	B	1643	TRP
1	B	1653	PHE
1	B	1658	LEU
1	B	1673	ASN
1	B	1689	VAL
1	B	1726	THR
1	B	1735	ILE
1	B	1777	LEU
1	B	1797	LEU
1	B	1804	VAL
1	B	1824	LYS
1	B	1838	ASP
1	B	1843	VAL
1	B	1852	THR
1	B	1884	LEU
1	B	1889	LEU
1	B	1916	LEU
1	B	1924	TRP
1	B	1928	SER
1	B	1960	GLN
1	B	2001	VAL
1	B	2003	VAL
1	B	2081	GLU
1	B	2086	TYR
1	B	2101	SER
1	B	2141	HIS
1	B	2142	GLN
1	B	2166	GLU
1	C	1508	VAL
1	C	1513	GLU
1	C	1514	LEU
1	C	1536	PHE
1	C	1546	GLU
1	C	1571	VAL
1	C	1575	GLU

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Mol	Chain	Res	Type
1	C	1602	GLU
1	C	1629	ILE
1	C	1638	LEU
1	C	1661	GLU
1	C	1676	LEU
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1770	VAL
1	C	1772	THR
1	C	1774	ASN
1	C	1781	GLN
1	C	1783	MET
1	C	1792	THR
1	C	1824	LYS
1	C	1898	THR
1	C	1911	ASN
1	C	1924	TRP
1	C	1926	PRO
1	C	1928	SER
1	C	1950	LEU
1	C	1968	LEU
1	C	1978	LEU
1	C	2001	VAL
1	C	2028	GLN
1	C	2037	ARG
1	C	2045	ASN
1	C	2084	PRO
1	C	2114	GLU
1	C	2129	ARG
1	C	2148	ARG
1	C	2186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1525	ASN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN

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Mol	Chain	Res	Type
1	A	1624	ASN
1	A	1644	ASN
1	A	1683	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1781	GLN
1	A	1786	ASN
1	A	1815	ASN
1	A	1901	ASN
1	A	1909	ASN
1	A	1922	GLN
1	A	1934	GLN
1	A	2008	ASN
1	A	2028	GLN
1	A	2092	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2141	HIS
1	A	2170	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1581	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1925	HIS
1	B	1934	GLN
1	B	1937	ASN
1	B	1941	ASN
1	B	1944	GLN
1	B	1960	GLN
1	B	2088	GLN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN

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Mol	Chain	Res	Type
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1581	GLN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1654	GLN
1	C	1744	GLN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1815	ASN
1	C	1837	ASN
1	C	1909	ASN
1	C	1911	ASN
1	C	1922	GLN
1	C	1934	GLN
1	C	1937	ASN
1	C	2011	GLN
1	C	2045	ASN
1	C	2092	GLN
1	C	2142	GLN
1	C	2170	GLN

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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B36	B	1	-	39,39,39	3.74	32 (82%)	56,56,56	1.28	4 (7%)
2	B36	C	1	-	39,39,39	3.55	27 (69%)	56,56,56	1.33	6 (10%)
2	B36	A	1	-	39,39,39	2.76	23 (58%)	56,56,56	1.46	10 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B36	B	1	-	-	2/12/22/22	0/6/6/6
2	B36	C	1	-	-	4/12/22/22	0/6/6/6
2	B36	A	1	-	-	1/12/22/22	0/6/6/6

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	B36	CAZ-CBE	6.63	1.50	1.41
2	C	1	B36	CAZ-CBF	6.62	1.50	1.41
2	C	1	B36	CBA-CBD	6.30	1.51	1.42
2	C	1	B36	CAX-NAV	6.27	1.45	1.33
2	A	1	B36	CAZ-CBE	6.03	1.50	1.41
2	B	1	B36	CAZ-CBF	5.67	1.49	1.41
2	B	1	B36	CAX-NAV	5.64	1.43	1.33
2	B	1	B36	CBE-CBB	5.55	1.53	1.43
2	A	1	B36	CAZ-CBF	5.39	1.49	1.41
2	B	1	B36	CAP-CBC	5.30	1.49	1.39
2	C	1	B36	CAF-CAL	5.11	1.47	1.36
2	B	1	B36	CAC-CAI	4.92	1.47	1.36
2	C	1	B36	CAE-CAK	4.88	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	B36	CAF-CAL	4.84	1.46	1.36
2	B	1	B36	CAE-CAK	4.79	1.46	1.36
2	C	1	B36	CAZ-CBE	4.77	1.48	1.41
2	C	1	B36	CAD-CAJ	4.62	1.46	1.36
2	B	1	B36	CAN-CAH	4.62	1.46	1.36
2	B	1	B36	CBF-CBC	4.56	1.51	1.43
2	B	1	B36	CAP-CBB	4.47	1.47	1.39
2	C	1	B36	CAN-CAH	4.39	1.46	1.36
2	C	1	B36	CAW-NBH	4.37	1.43	1.34
2	B	1	B36	CAZ-CAW	4.27	1.55	1.50
2	C	1	B36	CBE-CBB	4.19	1.50	1.43
2	A	1	B36	CBA-CBD	4.10	1.48	1.42
2	B	1	B36	CBA-CBD	4.10	1.48	1.42
2	B	1	B36	CBD-NAV	4.05	1.43	1.37
2	B	1	B36	CAD-CAJ	4.00	1.45	1.36
2	A	1	B36	CAW-NBH	3.94	1.43	1.34
2	C	1	B36	CAL-CBF	3.85	1.50	1.42
2	B	1	B36	CAC-CAE	3.83	1.46	1.38
2	C	1	B36	CAH-CAY	3.82	1.46	1.38
2	B	1	B36	CAW-NBH	3.81	1.42	1.34
2	B	1	B36	CAM-CAG	3.80	1.44	1.36
2	B	1	B36	CAH-CAY	3.80	1.46	1.38
2	C	1	B36	CBF-CBC	3.79	1.50	1.43
2	B	1	B36	CAO-CAY	3.77	1.46	1.37
2	C	1	B36	CAM-CAG	3.76	1.44	1.36
2	C	1	B36	CAC-CAI	3.75	1.44	1.36
2	C	1	B36	CAP-CBB	3.73	1.46	1.39
2	A	1	B36	CBE-CBB	3.69	1.49	1.43
2	C	1	B36	CAZ-CAW	3.64	1.54	1.50
2	A	1	B36	CAO-CAY	3.58	1.45	1.37
2	C	1	B36	CBD-NAV	3.52	1.43	1.37
2	A	1	B36	CAE-CAK	3.49	1.44	1.36
2	A	1	B36	CBF-CBC	3.46	1.49	1.43
2	C	1	B36	CAP-CBC	3.41	1.45	1.39
2	A	1	B36	CAS-NBH	3.31	1.53	1.47
2	C	1	B36	CAG-CAX	3.29	1.46	1.39
2	A	1	B36	CAF-CAL	3.28	1.43	1.36
2	A	1	B36	CAX-NAV	3.25	1.39	1.33
2	C	1	B36	CAF-CAD	3.21	1.45	1.38
2	B	1	B36	CAK-CBE	3.20	1.48	1.42
2	A	1	B36	CAN-CAH	3.13	1.43	1.36
2	A	1	B36	CAM-CAG	3.10	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	B36	CAO-CAY	3.09	1.44	1.37
2	A	1	B36	CAD-CAJ	3.08	1.43	1.36
2	A	1	B36	CAZ-CAW	3.07	1.53	1.50
2	A	1	B36	CAC-CAI	3.04	1.43	1.36
2	B	1	B36	CAF-CAD	3.02	1.44	1.38
2	B	1	B36	CAS-NBH	3.01	1.52	1.47
2	C	1	B36	CAC-CAE	2.99	1.44	1.38
2	C	1	B36	CAS-NBH	2.91	1.52	1.47
2	A	1	B36	CAH-CAY	2.87	1.44	1.38
2	B	1	B36	CAT-NBH	2.83	1.52	1.47
2	B	1	B36	CAL-CBF	2.79	1.47	1.42
2	B	1	B36	CAQ-CAS	2.60	1.59	1.52
2	A	1	B36	CAC-CAE	2.57	1.43	1.38
2	A	1	B36	CAF-CAD	2.52	1.43	1.38
2	B	1	B36	CAJ-CBC	2.52	1.47	1.42
2	B	1	B36	CAN-CBD	2.51	1.46	1.41
2	B	1	B36	CAR-CBG	2.48	1.59	1.52
2	B	1	B36	CAQ-CBG	2.46	1.59	1.52
2	A	1	B36	CBD-NAV	2.45	1.41	1.37
2	C	1	B36	CAU-CBG	2.40	1.61	1.53
2	C	1	B36	OAB-CAW	2.36	1.27	1.22
2	A	1	B36	CAP-CBC	2.33	1.43	1.39
2	A	1	B36	CAP-CBB	2.28	1.43	1.39
2	B	1	B36	CAI-CBB	2.13	1.46	1.42
2	C	1	B36	CAQ-CBG	2.07	1.58	1.52
2	B	1	B36	CAM-CBA	2.05	1.46	1.42
2	A	1	B36	CAL-CBF	2.05	1.46	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	B36	CAN-CBD-NAV	4.01	124.55	118.69
2	A	1	B36	CBE-CAZ-CAW	3.90	122.87	119.27
2	B	1	B36	CBA-CBD-NAV	-3.66	117.21	122.25
2	C	1	B36	CAN-CBD-NAV	3.47	123.75	118.69
2	A	1	B36	CBA-CBD-NAV	-3.42	117.55	122.25
2	A	1	B36	CAN-CBD-NAV	3.41	123.67	118.69
2	C	1	B36	CBE-CAZ-CAW	3.40	122.40	119.27
2	A	1	B36	CAZ-CAW-NBH	3.05	121.13	117.76
2	C	1	B36	CBA-CBD-NAV	-2.89	118.27	122.25
2	A	1	B36	CBF-CAZ-CBE	-2.88	117.27	120.86
2	A	1	B36	CAI-CBB-CAP	-2.57	117.92	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	B36	CAJ-CBC-CAP	-2.46	118.09	122.00
2	C	1	B36	CAI-CBB-CAP	-2.30	118.36	122.00
2	C	1	B36	CAM-CBA-CAO	-2.19	118.24	122.00
2	A	1	B36	OAB-CAW-CAZ	-2.18	118.70	121.50
2	B	1	B36	CAX-NAV-CBD	2.16	122.32	118.27
2	B	1	B36	CAO-CBA-CBD	2.08	120.97	118.31
2	A	1	B36	CAX-NAV-CBD	2.04	122.08	118.27
2	A	1	B36	CAP-CBC-CBF	2.03	121.42	119.28
2	C	1	B36	CAO-CBA-CBD	2.00	120.88	118.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

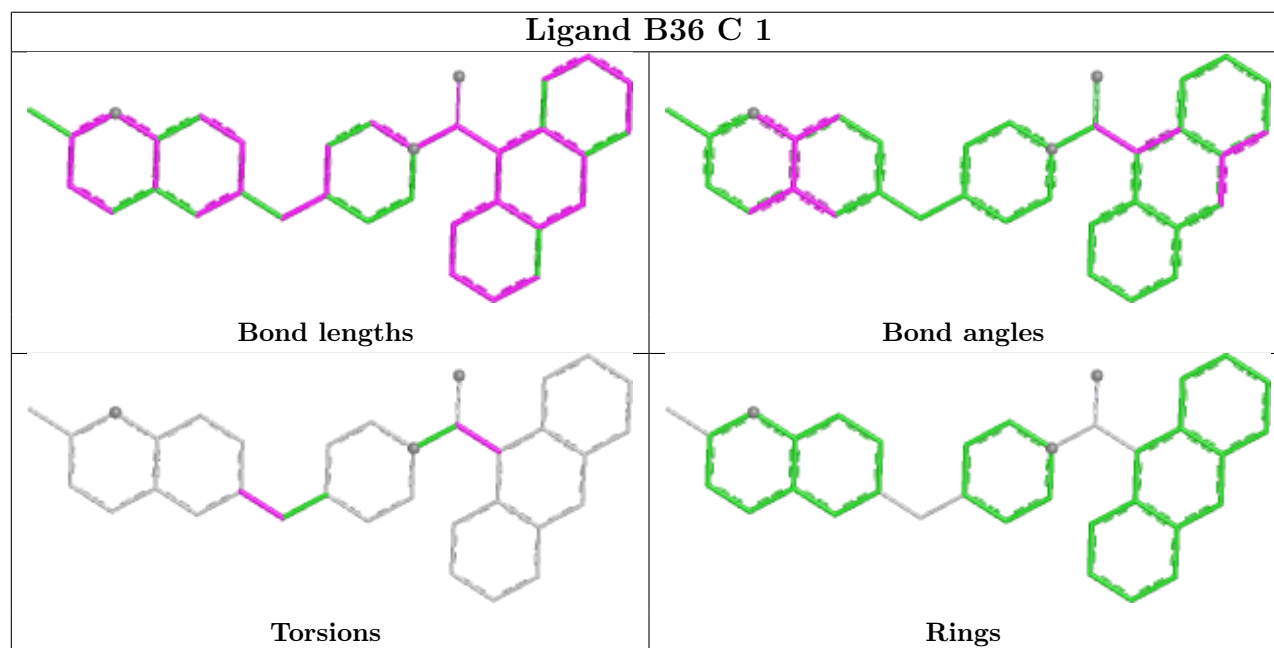
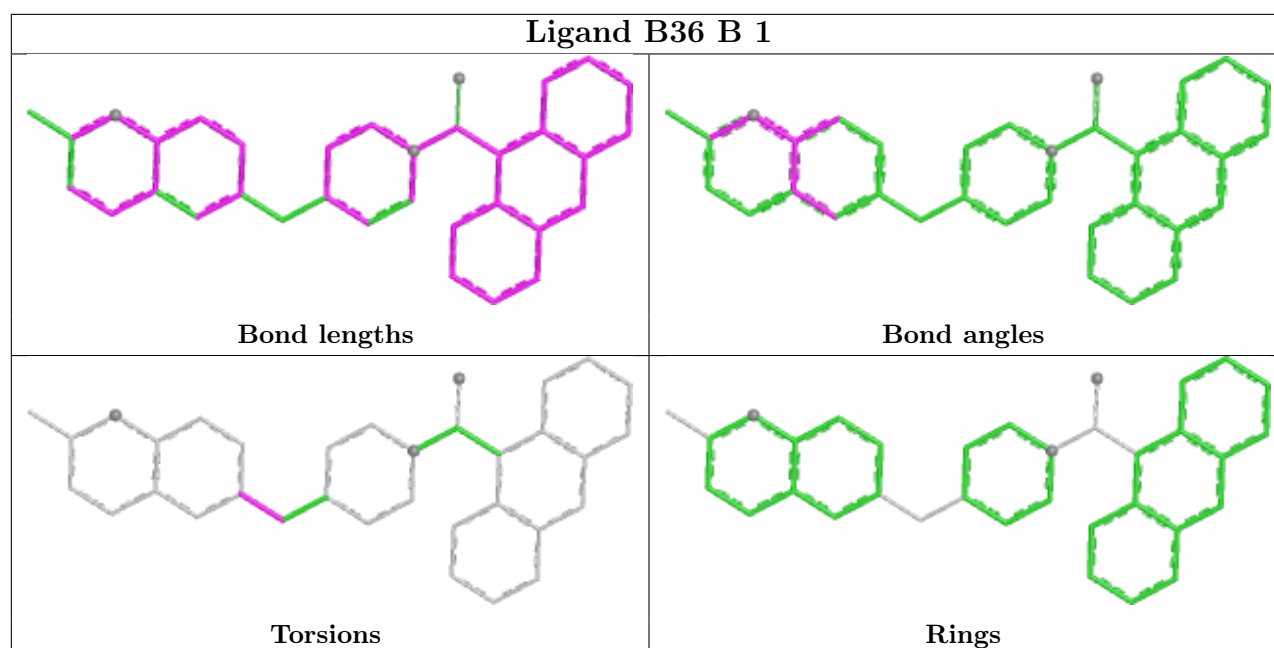
Mol	Chain	Res	Type	Atoms
2	B	1	B36	CBG-CAU-CAY-CAO
2	C	1	B36	CBG-CAU-CAY-CAO
2	B	1	B36	CBG-CAU-CAY-CAH
2	C	1	B36	CBG-CAU-CAY-CAH
2	A	1	B36	CBG-CAU-CAY-CAO
2	C	1	B36	NBH-CAW-CAZ-CBE
2	C	1	B36	NBH-CAW-CAZ-CBF

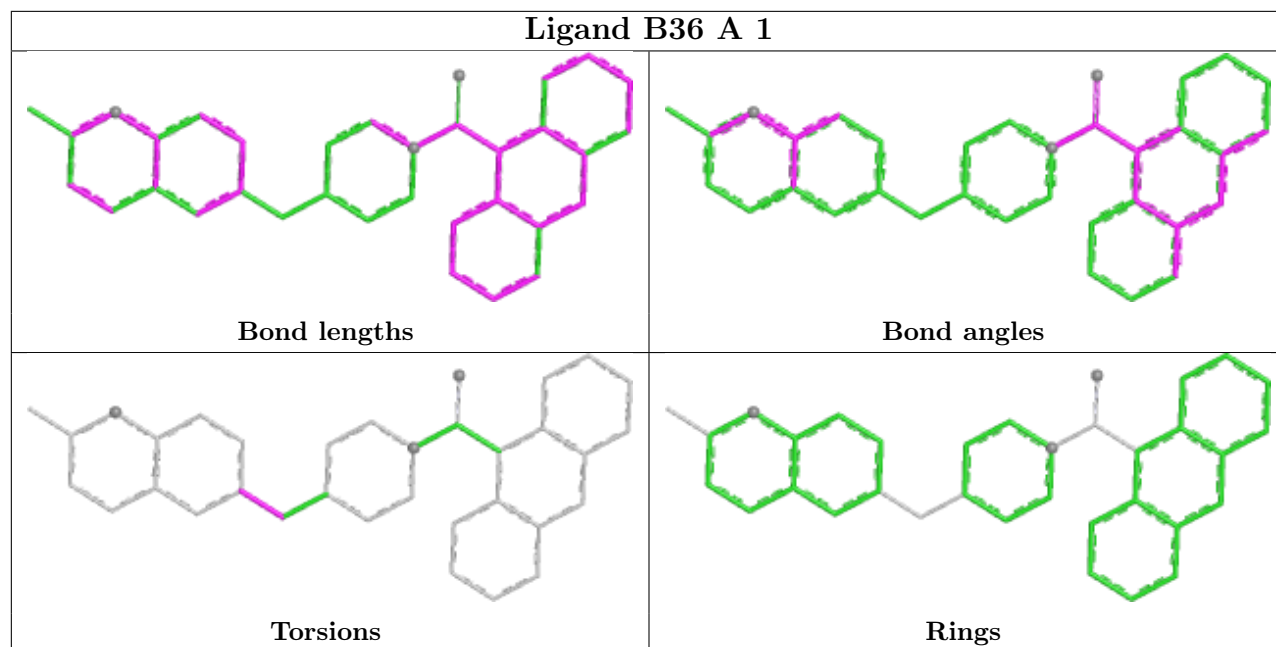
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	B36	2	0
2	C	1	B36	1	0
2	A	1	B36	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	681/769 (88%)	0.23	40 (5%) 28 21	24, 43, 89, 107	0
1	B	675/769 (87%)	0.36	63 (9%) 14 10	22, 46, 102, 119	0
1	C	665/769 (86%)	0.32	67 (10%) 12 9	23, 46, 111, 132	0
All	All	2021/2307 (87%)	0.30	170 (8%) 17 12	22, 45, 99, 132	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2047	LEU	11.2
1	B	2047	LEU	9.5
1	A	2047	LEU	8.4
1	B	2189	LEU	8.0
1	A	2195	ALA	7.5
1	C	2143	VAL	6.2
1	B	2143	VAL	6.1
1	C	1646	ALA	6.0
1	A	2194	PHE	5.7
1	C	2081	GLU	5.5
1	A	2144	GLY	5.3
1	A	2191	LEU	5.3
1	B	2082	LEU	5.2
1	B	2085	ILE	5.1
1	A	2037	ARG	5.0
1	B	1681	VAL	4.9
1	A	1482	PRO	4.9
1	A	2193	SER	4.9
1	C	1684	GLY	4.8
1	A	2143	VAL	4.8
1	C	1681	VAL	4.8
1	A	1681	VAL	4.7
1	A	1680	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	2189	LEU	4.6
1	C	1682	ILE	4.5
1	C	1669	PHE	4.4
1	B	2083	LEU	4.4
1	C	2045	ASN	4.3
1	C	1648	ASN	4.3
1	C	1655	TYR	4.3
1	B	2041	LEU	4.2
1	C	1685	GLU	4.2
1	B	2043	THR	4.1
1	B	1682	ILE	4.1
1	C	1643	TRP	4.1
1	B	2145	GLU	4.1
1	A	2081	GLU	4.0
1	C	1671	LYS	4.0
1	C	1667	LYS	3.9
1	B	1684	GLY	3.8
1	A	1685	GLU	3.8
1	C	1660	SER	3.8
1	A	2082	LEU	3.8
1	B	1646	ALA	3.7
1	C	2037	ARG	3.7
1	C	2046	ARG	3.7
1	B	2188	GLY	3.6
1	C	2085	ILE	3.6
1	B	2046	ARG	3.6
1	C	1679	ARG	3.5
1	B	2187	LYS	3.5
1	B	2081	GLU	3.5
1	B	2037	ARG	3.5
1	C	1647	ALA	3.5
1	C	1668	LYS	3.4
1	C	1680	THR	3.4
1	C	1654	GLN	3.3
1	C	2082	LEU	3.3
1	B	2036	ARG	3.3
1	C	2141	HIS	3.2
1	B	1680	THR	3.2
1	A	1682	ILE	3.2
1	B	2141	HIS	3.2
1	B	1651	LYS	3.2
1	B	1824	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1679	ARG	3.2
1	B	2086	TYR	3.1
1	C	1657	TYR	3.1
1	B	1678	GLU	3.1
1	B	1822	GLU	3.1
1	B	1839	GLU	3.1
1	B	2044	MET	3.0
1	B	1667	LYS	3.0
1	C	1661	GLU	2.9
1	A	2046	ARG	2.9
1	C	1687	ARG	2.9
1	C	1683	ASN	2.9
1	C	2041	LEU	2.9
1	B	2179	TYR	2.9
1	A	2190	LYS	2.9
1	B	2185	LYS	2.9
1	C	1531	LYS	2.9
1	B	2032	GLY	2.8
1	C	1675	VAL	2.8
1	A	1643	TRP	2.8
1	B	2180	LYS	2.8
1	C	2043	THR	2.8
1	A	1494	GLN	2.8
1	A	2154	ARG	2.8
1	B	1683	ASN	2.8
1	B	2039	LYS	2.8
1	C	1644	ASN	2.7
1	C	1651	LYS	2.7
1	B	1648	ASN	2.7
1	B	2045	ASN	2.7
1	A	1645	ASP	2.7
1	A	1684	GLY	2.7
1	C	1670	ASP	2.7
1	B	2142	GLN	2.7
1	C	2028	GLN	2.7
1	B	1647	ALA	2.7
1	C	1688	PHE	2.7
1	C	1638	LEU	2.7
1	B	2084	PRO	2.7
1	B	1649	PRO	2.6
1	A	2192	GLU	2.6
1	C	2044	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2042	ASP	2.6
1	B	1482	PRO	2.6
1	A	1769	GLU	2.6
1	B	2028	GLN	2.6
1	C	1686	GLU	2.6
1	C	1650	ASP	2.5
1	C	1629	ILE	2.5
1	C	2142	GLN	2.5
1	C	1658	LEU	2.5
1	C	2042	ASP	2.5
1	C	1516	ARG	2.5
1	C	1636	VAL	2.4
1	C	2144	GLY	2.4
1	A	1837	ASN	2.4
1	C	1649	PRO	2.4
1	B	1669	PHE	2.4
1	B	2144	GLY	2.4
1	C	1652	GLY	2.4
1	C	1665	THR	2.4
1	B	2149	LEU	2.4
1	C	1645	ASP	2.3
1	A	1686	GLU	2.3
1	B	1686	GLU	2.3
1	B	1640	GLN	2.3
1	B	1660	SER	2.3
1	B	1643	TRP	2.3
1	B	1853	GLU	2.3
1	C	1911	ASN	2.3
1	B	1661	GLU	2.3
1	C	1641	VAL	2.2
1	A	1650	ASP	2.2
1	A	2036	ARG	2.2
1	B	1655	TYR	2.2
1	B	2035	PHE	2.2
1	A	2141	HIS	2.2
1	C	1659	THR	2.2
1	C	1662	GLY	2.2
1	B	1679	ARG	2.2
1	A	1646	ALA	2.2
1	C	1914	GLU	2.2
1	B	1659	THR	2.1
1	A	2148	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1690	ILE	2.1
1	B	1837	ASN	2.1
1	C	1837	ASN	2.1
1	B	1530	VAL	2.1
1	B	1650	ASP	2.1
1	B	1662	GLY	2.1
1	C	1533	THR	2.1
1	A	1655	TYR	2.1
1	A	2086	TYR	2.1
1	A	1649	PRO	2.1
1	A	1683	ASN	2.1
1	A	1653	PHE	2.1
1	C	1910	PRO	2.1
1	C	1630	GLY	2.1
1	B	2158	TRP	2.1
1	A	1855	GLY	2.0
1	A	1651	LYS	2.0
1	C	1689	VAL	2.0
1	C	2149	LEU	2.0
1	B	2038	GLU	2.0
1	C	1530	VAL	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.

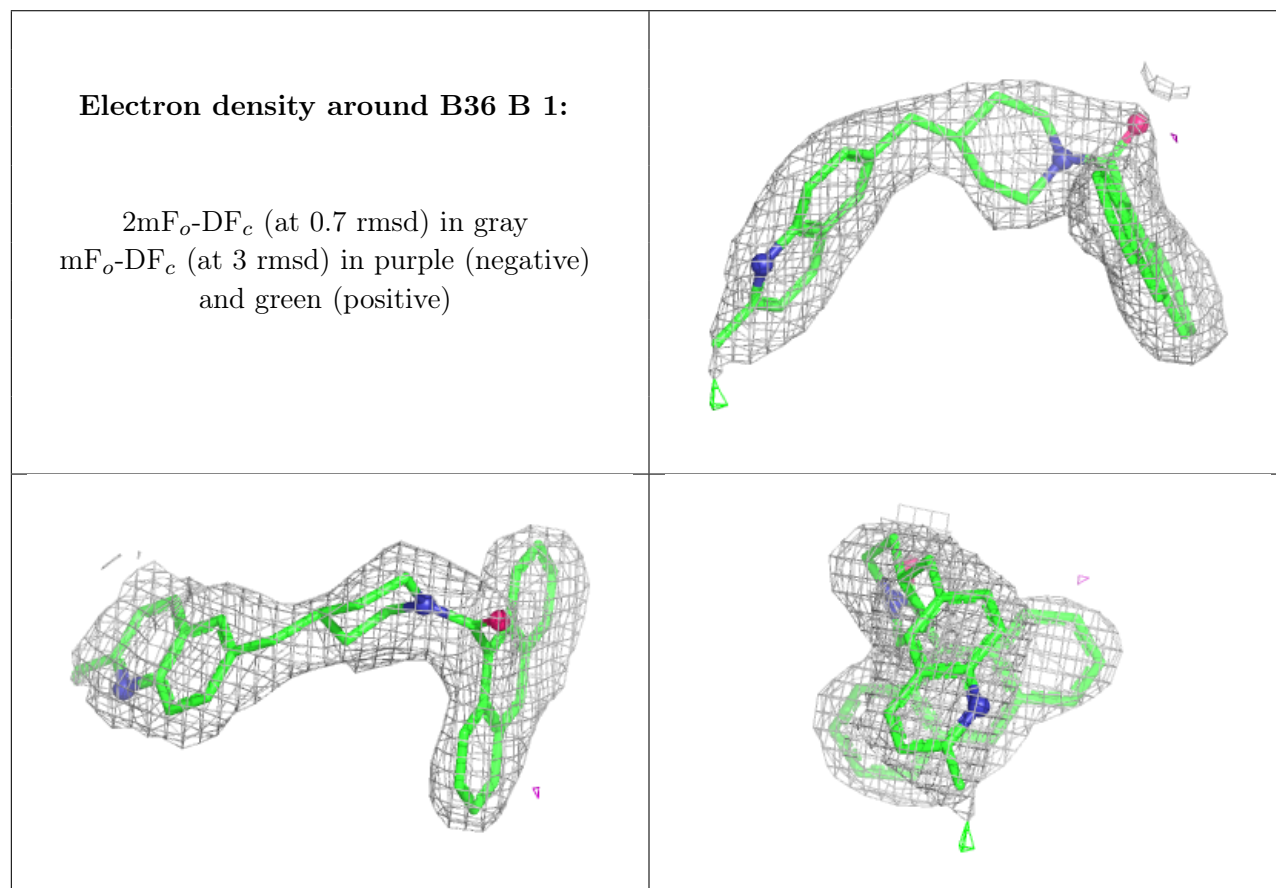
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B36	B	1	34/34	0.89	0.19	63,68,71,72	0
2	B36	A	1	34/34	0.90	0.19	65,70,74,74	0

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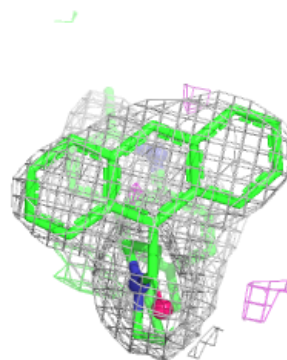
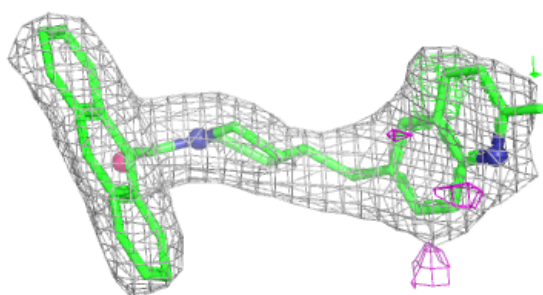
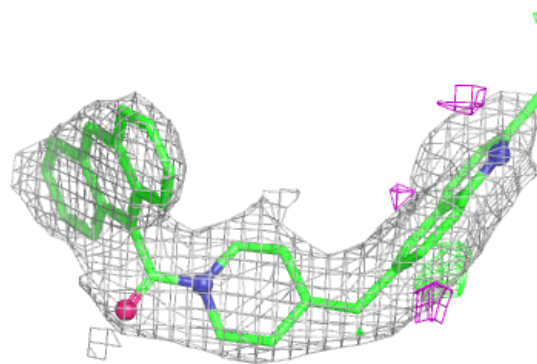
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B36	C	1	34/34	0.92	0.17	59,61,63,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

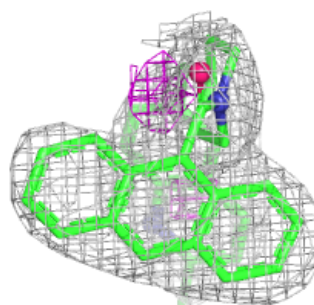
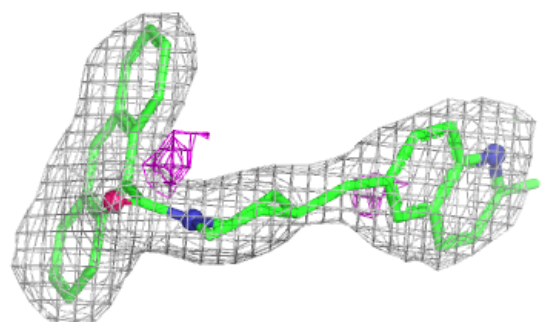
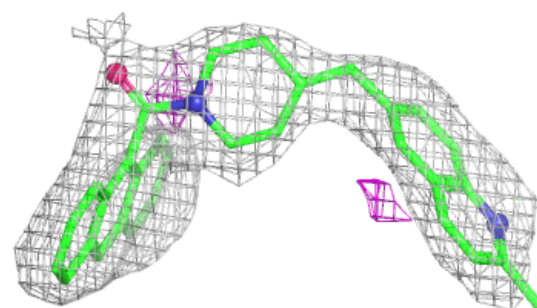


Electron density around B36 A 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B36 C 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.