



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:39 AM UTC

PDB ID : 1OD2 / pdb_00001od2
Title : Acetyl-CoA Carboxylase Carboxyltransferase Domain
Authors : Zhang, H.; Yang, Z.; Shen, Y.; Tong, L.
Deposited on : 2003-02-12
Resolution : 2.70 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

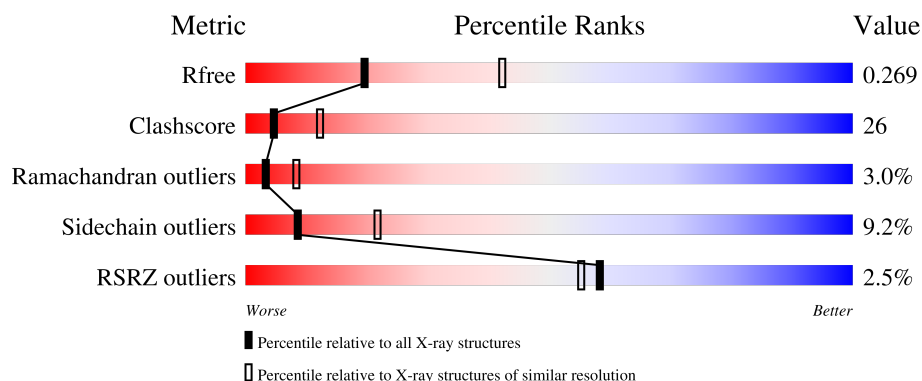
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

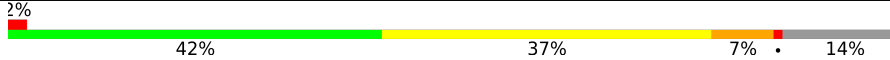
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	805	
1	B	805	

2 Entry composition [i](#)

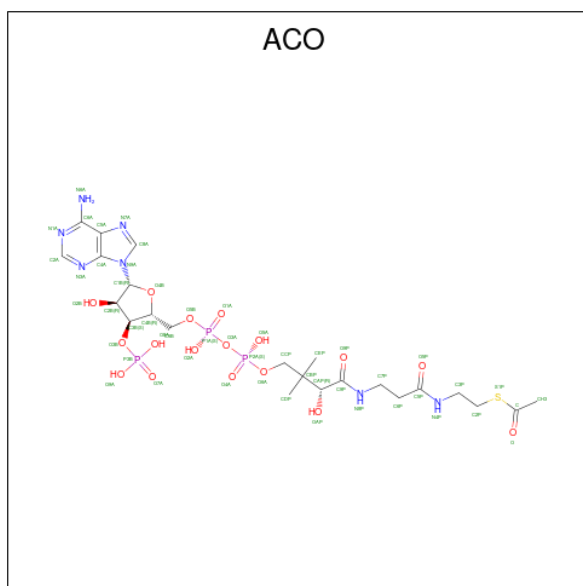
There are 4 unique types of molecules in this entry. The entry contains 11433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-COENZYME A CARBOXYLASE.

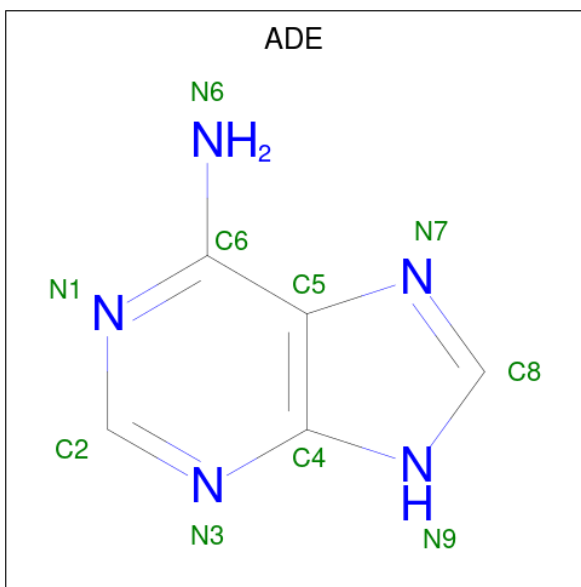
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	Se	0	0	1
			5742	3650	994	1079	2	17			
1	B	696	Total	C	N	O	S	Se	0	0	1
			5544	3518	963	1044	2	17			

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is ADENINE (CCD ID: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			10	5	5		

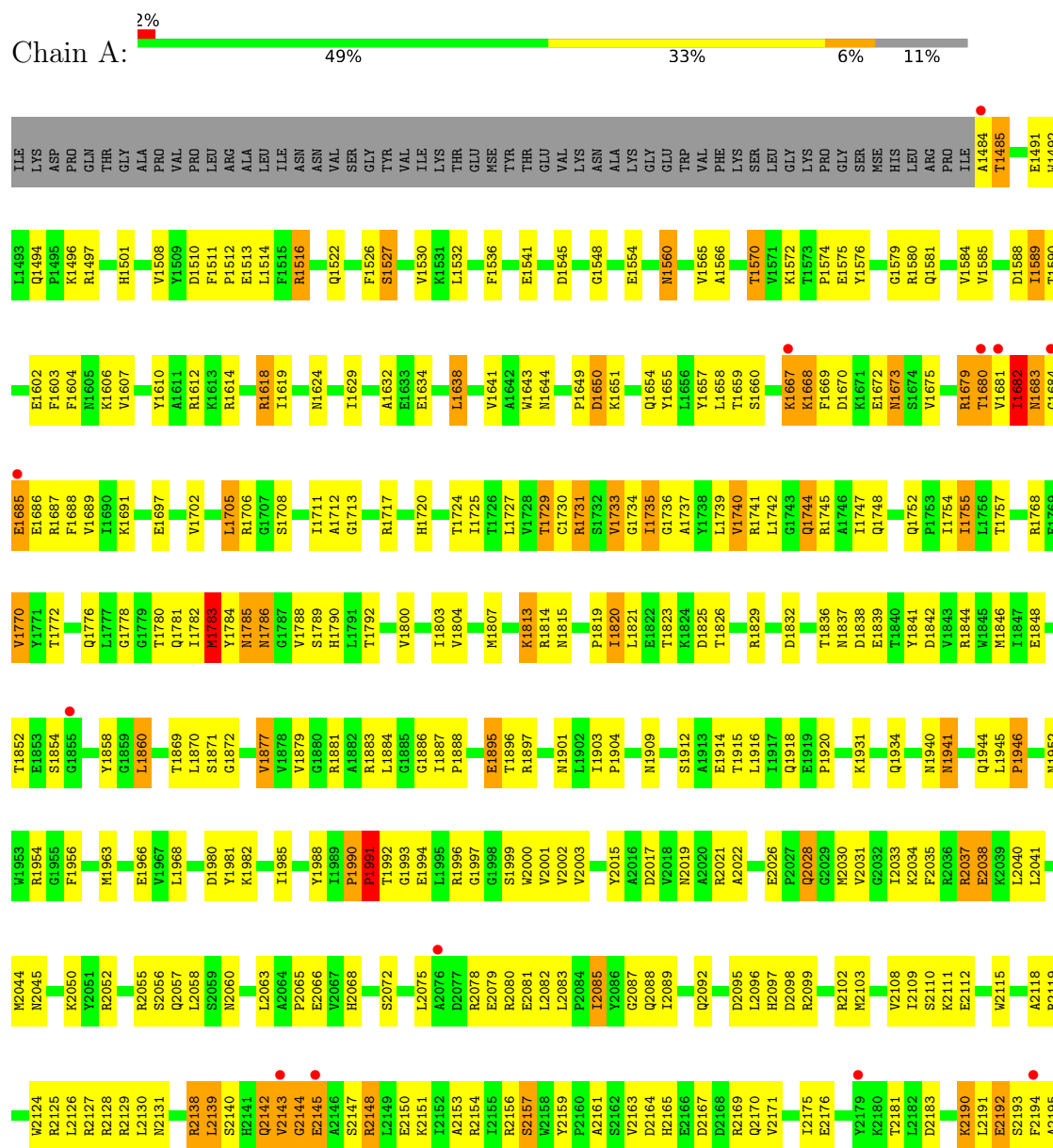
- Molecule 4 is water.

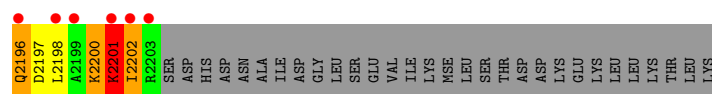
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	42	Total	O	0	0
			42	42		

3 Residue-property plots

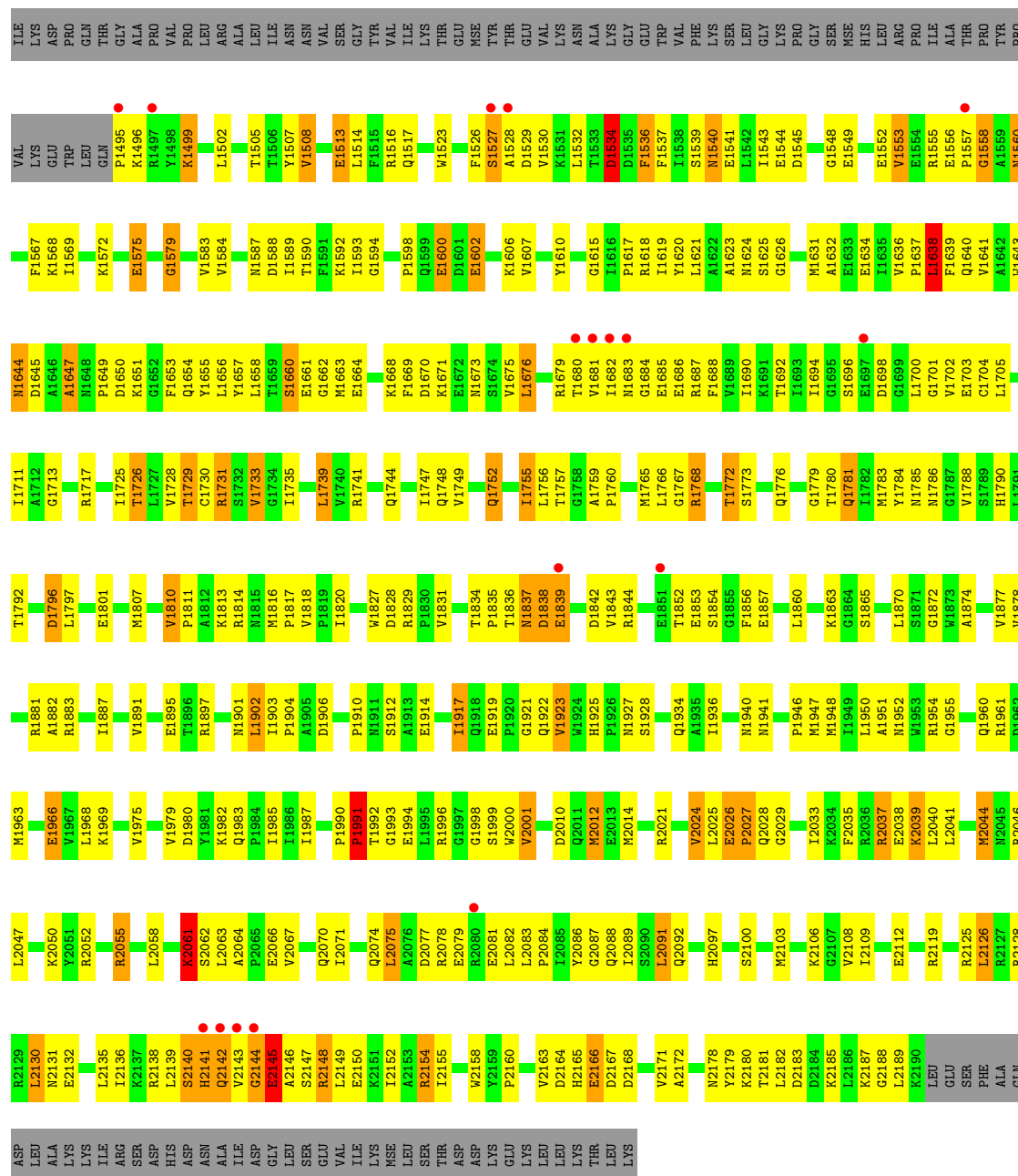
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-COENZYME A CARBOXYLASE





Molecule 1: ACETYL-COENZYME A CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.87Å 138.13Å 101.40Å 90.00° 114.42° 90.00°	Depositor
Resolution (Å)	28.85 – 2.70 28.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.85-2.70) 93.1 (28.85-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.279 0.217 , 0.269	Depositor DCC
R_{free} test set	6032 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11433	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: ADE, ACO

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	0.53	1/5850 (0.0%)	1.01	25/7893 (0.3%)
1	B	0.53	0/5646	1.01	31/7615 (0.4%)
All	All	0.53	1/11496 (0.0%)	1.01	56/15508 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2202	ILE	C-N	-5.15	1.26	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1941	ASN	N-CA-C	10.34	123.64	111.02
1	A	2201	LYS	N-CA-C	-9.37	100.09	113.21
1	B	1941	ASN	N-CA-C	9.09	121.11	111.03
1	B	1966	GLU	N-CA-C	7.36	121.56	112.58
1	A	1946	PRO	N-CA-C	-7.32	100.22	111.13
1	B	1600	GLU	N-CA-C	-7.10	103.54	111.28
1	A	1638	LEU	N-CA-C	6.87	120.92	111.71
1	B	1644	ASN	N-CA-C	-6.83	103.92	111.36
1	B	2112	GLU	N-CA-C	-6.76	99.57	110.32
1	A	1914	GLU	N-CA-C	-6.68	100.81	110.24
1	A	2157	SER	N-CA-C	-6.61	105.22	113.28
1	A	1755	ILE	N-CA-C	6.51	118.31	108.80
1	B	1660	SER	N-CA-C	-6.47	104.08	112.23
1	B	1676	LEU	N-CA-C	-6.33	98.95	109.46
1	B	1579	GLY	N-CA-C	6.22	119.25	112.29
1	B	1502	LEU	N-CA-C	-6.15	104.66	111.36
1	B	2154	ARG	N-CA-C	-6.05	104.80	111.82
1	B	1946	PRO	N-CA-C	-6.02	100.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1996	ARG	N-CA-C	5.97	119.40	109.96
1	B	1752	GLN	CA-C-N	5.96	125.92	119.78
1	B	1752	GLN	C-N-CA	5.96	125.92	119.78
1	A	1990	PRO	CA-C-N	5.96	127.28	119.84
1	A	1990	PRO	C-N-CA	5.96	127.28	119.84
1	B	2087	GLY	N-CA-C	-5.90	105.46	113.37
1	B	1536	PHE	N-CA-C	-5.90	106.04	113.18
1	B	1796	ASP	N-CA-C	5.88	118.44	111.33
1	B	2172	ALA	N-CA-C	-5.86	104.81	111.07
1	A	1644	ASN	N-CA-C	-5.81	104.54	111.69
1	A	1945	LEU	N-CA-C	5.79	119.31	110.50
1	A	1536	PHE	N-CA-C	-5.76	106.09	113.23
1	A	1729	THR	N-CA-C	5.71	120.52	113.50
1	A	1685	GLU	N-CA-C	5.70	116.92	108.60
1	B	2012	MSE	N-CA-C	5.64	118.87	110.52
1	B	1636	VAL	CA-C-N	-5.51	114.22	120.89
1	B	1636	VAL	C-N-CA	-5.51	114.22	120.89
1	B	1639	PHE	N-CA-C	5.43	118.52	110.48
1	A	2087	GLY	N-CA-C	-5.42	106.23	112.73
1	A	1492	TRP	N-CA-C	-5.35	105.57	112.68
1	A	1516	ARG	N-CA-C	-5.33	105.12	111.03
1	B	1647	ALA	N-CA-C	-5.32	101.02	109.96
1	A	2148	ARG	N-CA-C	-5.31	105.39	111.07
1	A	1966	GLU	N-CA-C	5.28	118.86	111.74
1	A	1954	ARG	N-CA-C	-5.26	106.63	113.16
1	B	1733	VAL	N-CA-C	5.25	115.47	108.11
1	B	2075	LEU	N-CA-C	-5.25	105.23	111.69
1	B	2033	ILE	CB-CA-C	-5.24	106.46	111.44
1	B	1729	THR	N-CA-C	5.22	119.74	112.90
1	A	1940	ASN	N-CA-C	5.15	117.88	111.24
1	A	1871	SER	N-CA-C	5.14	118.66	112.38
1	B	1919	GLU	CA-C-N	5.12	125.05	119.78
1	B	1919	GLU	C-N-CA	5.12	125.05	119.78
1	B	1696	SER	N-CA-C	-5.11	107.60	113.88
1	A	2112	GLU	N-CA-C	-5.06	102.03	110.17
1	A	1783	MSE	N-CA-C	5.05	117.51	111.71
1	B	1638	LEU	N-CA-C	5.03	119.68	113.50
1	A	1770	VAL	N-CA-C	5.00	115.23	110.53

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	5742	0	5688	286	0
1	B	5544	0	5483	330	0
2	A	48	0	31	4	0
3	B	10	0	4	0	0
4	A	47	0	0	1	0
4	B	42	0	0	2	0
All	All	11433	0	11206	585	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 26.

All (585) 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:2085:ILE:H	1:A:2085:ILE:HD12	1.17	1.06
1:A:2085:ILE:HG12	1:B:1650:ASP:HA	1.38	1.01
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.18	0.99
1:A:2034:LYS:HB2	1:B:1631:MSE:HE3	1.48	0.96
1:B:1940:ASN:HD22	1:B:1983:GLN:HE22	1.07	0.94
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	1.82	0.93
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.11	0.89
1:A:1570:THR:HB	1:A:1581:GLN:HG2	1.52	0.87
1:B:1772:THR:H	1:B:1776:GLN:NE2	1.73	0.87
1:B:1940:ASN:HD22	1:B:1983:GLN:NE2	1.75	0.85
1:B:1860:LEU:CD2	1:B:1948:MSE:HE1	2.06	0.85
1:A:2065:PRO:HG2	1:A:2066:GLU:OE2	1.75	0.84
1:B:1991:PRO:O	1:B:1993:GLY:N	2.09	0.84
1:A:2037:ARG:HH11	1:A:2037:ARG:HB3	1.39	0.84
1:A:1629:ILE:HG22	1:B:2024:VAL:HG11	1.60	0.84
1:A:1679:ARG:HG2	1:A:1680:THR:N	1.93	0.83
1:B:1772:THR:H	1:B:1776:GLN:HE22	1.25	0.83
1:A:1782:ILE:O	1:A:1786:ASN:HB2	1.81	0.81
1:A:2034:LYS:CB	1:B:1631:MSE:HE3	2.10	0.81
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.62	0.81
1:B:1829:ARG:CZ	1:B:2119:ARG:HE	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2092:GLN:O	1:A:2096:LEU:HD23	1.81	0.81
1:B:2070:GLN:HE21	1:B:2074:GLN:HE21	1.29	0.81
1:A:2085:ILE:H	1:A:2085:ILE:CD1	1.94	0.81
1:B:1499:LYS:HE2	1:B:1590:THR:HB	1.60	0.81
1:B:1644:ASN:HD21	1:B:1654:GLN:HE21	1.25	0.80
1:A:1783:MSE:HE1	1:B:1963:MSE:HE3	1.62	0.79
1:B:1940:ASN:ND2	1:B:1983:GLN:HE22	1.81	0.79
1:A:1667:LYS:C	1:A:1669:PHE:H	1.91	0.78
1:B:2106:LYS:HE2	1:B:2106:LYS:HA	1.66	0.78
1:A:2031:VAL:HG13	1:A:2035:PHE:HB3	1.66	0.77
2:A:3203:ACO:O4A	2:A:3203:ACO:H10	1.84	0.77
1:B:2146:ALA:HB1	1:B:2150:GLU:OE2	1.84	0.77
1:B:2142:GLN:HE22	1:B:2144:GLY:N	1.84	0.75
1:A:1786:ASN:ND2	1:B:1966:GLU:HG3	2.00	0.75
1:B:1725:ILE:HD11	1:B:1747:ILE:HD11	1.69	0.75
1:B:2077:ASP:O	1:B:2081:GLU:HG3	1.85	0.74
1:B:1539:SER:C	1:B:1540:ASN:HD22	1.95	0.74
1:B:1860:LEU:HD21	1:B:1948:MSE:HE1	1.68	0.74
1:A:1785:ASN:HD22	1:A:1785:ASN:N	1.85	0.74
1:B:1657:TYR:CD2	1:B:1687:ARG:HB2	2.23	0.73
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.53	0.73
1:B:2070:GLN:HE21	1:B:2074:GLN:NE2	1.86	0.73
1:A:2142:GLN:HB3	1:A:2190:LYS:CE	2.19	0.73
1:A:1679:ARG:HG2	1:A:1680:THR:H	1.54	0.72
1:A:2079:GLU:O	1:A:2083:LEU:HB2	1.89	0.72
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.70	0.72
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.70	0.72
1:B:1499:LYS:HG2	1:B:1590:THR:HG22	1.71	0.71
1:B:1658:LEU:HG	1:B:1690:ILE:HD11	1.70	0.71
1:B:1921:GLY:O	1:B:1923:VAL:HG12	1.91	0.71
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	1.89	0.71
1:B:1766:LEU:O	1:B:1768:ARG:HG2	1.91	0.71
1:B:2046:ARG:CZ	1:B:2047:LEU:HD11	2.21	0.71
1:A:2200:LYS:HA	1:A:2200:LYS:HZ3	1.55	0.70
1:B:1954:ARG:HG3	1:B:1954:ARG:HH11	1.55	0.70
1:A:1560:ASN:H	1:A:1560:ASN:ND2	1.80	0.70
1:A:2080:ARG:O	1:A:2080:ARG:HG2	1.92	0.69
1:A:2142:GLN:HB3	1:A:2190:LYS:HE3	1.74	0.69
1:B:2070:GLN:NE2	1:B:2074:GLN:HE21	1.91	0.69
1:A:1838:ASP:HB2	1:A:1839:GLU:OE1	1.91	0.69
1:A:2191:LEU:HD23	1:A:2191:LEU:C	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1731:ARG:HH12	2:A:3203:ACO:H121	1.58	0.69
1:B:2010:ASP:CG	1:B:2148:ARG:HG3	2.18	0.69
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.40	0.68
1:B:2167:ASP:O	1:B:2171:VAL:HG23	1.93	0.68
1:B:1773:SER:H	1:B:1776:GLN:HE21	1.42	0.68
1:B:2142:GLN:HE22	1:B:2144:GLY:CA	2.06	0.68
1:B:2125:ARG:NH1	1:B:2168:ASP:OD1	2.27	0.68
1:A:1682:ILE:C	1:A:1684:GLY:H	2.01	0.68
1:A:2033:ILE:HG22	1:A:2034:LYS:HG3	1.75	0.67
1:B:1634:GLU:O	1:B:1638:LEU:HD22	1.94	0.67
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.29	0.67
1:B:1768:ARG:HH11	1:B:1768:ARG:HB2	1.58	0.67
1:A:1733:VAL:HG13	1:A:1755:ILE:HG13	1.76	0.67
1:A:1735:ILE:HD12	1:A:1735:ILE:H	1.60	0.67
1:B:1701:GLY:O	1:B:1704:CYS:HB2	1.95	0.67
1:A:1731:ARG:NH1	2:A:3203:ACO:H121	2.09	0.66
1:A:2200:LYS:HZ1	1:A:2202:ILE:HB	1.61	0.66
1:A:1513:GLU:OE2	1:A:1516:ARG:NH1	2.28	0.66
1:B:2039:LYS:NZ	1:B:2039:LYS:HB2	2.10	0.66
1:A:2147:SER:OG	1:A:2150:GLU:HG3	1.95	0.66
1:B:1540:ASN:HD22	1:B:1540:ASN:N	1.94	0.65
1:A:1820:ILE:HD12	1:A:1886:GLY:C	2.21	0.65
1:B:1733:VAL:HG22	1:B:1755:ILE:HD11	1.79	0.65
1:A:1650:ASP:OD2	1:A:1650:ASP:N	2.30	0.65
1:A:1733:VAL:HA	1:A:1755:ILE:O	1.97	0.65
1:B:1685:GLU:HG2	1:B:1686:GLU:H	1.62	0.65
1:B:1991:PRO:C	1:B:1993:GLY:H	2.03	0.65
1:B:1637:PRO:HG2	1:B:1638:LEU:HD13	1.80	0.64
1:B:1836:THR:HB	1:B:1839:GLU:OE2	1.97	0.64
1:A:2096:LEU:HD12	1:B:1692:THR:HA	1.80	0.64
1:B:2055:ARG:HG3	1:B:2055:ARG:HH11	1.63	0.64
1:B:1541:GLU:HG3	1:B:1567:PHE:HE2	1.63	0.64
1:B:2142:GLN:NE2	1:B:2144:GLY:N	2.46	0.64
1:A:1679:ARG:HG3	1:A:1679:ARG:HH11	1.62	0.64
1:A:2089:ILE:HD13	1:B:1641:VAL:HG21	1.80	0.63
1:A:1603:PHE:O	1:A:1607:VAL:HG23	1.99	0.63
1:A:1680:THR:HG22	1:A:1687:ARG:HB2	1.80	0.63
1:A:2041:LEU:HD12	1:A:2044:MSE:HE3	1.81	0.62
1:B:1780:THR:O	1:B:1784:TYR:HB3	1.97	0.62
1:B:2188:GLY:O	1:B:2189:LEU:HD23	1.99	0.62
1:A:1790:HIS:HB3	1:A:1869:THR:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2138:ARG:HH11	1:A:2138:ARG:HB3	1.64	0.62
1:B:1749:VAL:O	1:B:1752:GLN:HB2	1.99	0.62
1:A:2193:SER:C	1:A:2195:ALA:H	2.07	0.62
1:A:1641:VAL:HG21	1:B:2089:ILE:HD13	1.82	0.62
1:B:1755:ILE:HD13	1:B:1755:ILE:H	1.64	0.62
1:B:1813:LYS:HG3	1:B:1816:MSE:HG3	1.80	0.62
1:B:1552:GLU:O	1:B:1553:VAL:HG13	2.00	0.62
1:B:2064:ALA:HB3	1:B:2067:VAL:HG23	1.80	0.62
1:A:1629:ILE:HG22	1:B:2024:VAL:CG1	2.28	0.61
1:A:1712:ALA:O	1:A:1742:LEU:HD13	2.00	0.61
1:A:2200:LYS:HE2	1:A:2202:ILE:HD12	1.82	0.61
1:B:1779:GLY:HA3	1:B:1781:GLN:OE1	2.00	0.61
1:B:1543:ILE:HD12	1:B:1544:GLU:O	2.00	0.61
1:B:1813:LYS:HG3	1:B:1816:MSE:CG	2.31	0.61
1:A:2057:GLN:O	1:A:2063:LEU:HD11	2.01	0.61
1:A:2142:GLN:HB3	1:A:2190:LYS:NZ	2.15	0.61
1:A:2142:GLN:CD	1:A:2143:VAL:H	2.09	0.61
1:B:1860:LEU:HD23	1:B:1948:MSE:HE1	1.82	0.61
1:A:2139:LEU:O	1:A:2151:LYS:HD3	2.00	0.60
1:A:1589:ILE:HD13	1:A:1589:ILE:O	2.02	0.60
1:A:2142:GLN:CD	1:A:2143:VAL:N	2.59	0.60
1:B:1966:GLU:HG2	1:B:1969:LYS:HE3	1.82	0.60
1:B:1572:LYS:HA	1:B:1579:GLY:HA2	1.83	0.60
1:B:2139:LEU:HD11	1:B:2154:ARG:NH1	2.17	0.59
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.50	0.59
1:A:2099:ARG:HG3	1:A:2099:ARG:HH11	1.67	0.59
1:B:1810:VAL:HG23	1:B:1811:PRO:HD2	1.84	0.59
1:A:2045:ASN:HD22	1:A:2055:ARG:HG3	1.68	0.59
1:B:1990:PRO:O	1:B:1991:PRO:O	2.20	0.59
1:A:1585:VAL:HG22	1:A:1607:VAL:HG11	1.84	0.59
1:A:1491:GLU:OE2	1:A:1501:HIS:HD2	1.86	0.59
1:B:1516:ARG:HH22	1:B:1534:ASP:HA	1.68	0.59
1:B:1772:THR:N	1:B:1776:GLN:NE2	2.49	0.59
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.03	0.59
1:A:2035:PHE:HB2	1:B:1631:MSE:HE1	1.84	0.58
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.85	0.58
1:B:2164:ASP:C	1:B:2166:GLU:H	2.11	0.58
1:B:1679:ARG:CZ	1:B:1686:GLU:OE1	2.51	0.58
1:B:2025:LEU:HD12	1:B:2029:GLY:HA3	1.84	0.58
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.04	0.58
1:A:1682:ILE:O	1:A:1684:GLY:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1755:ILE:HD13	1:B:1755:ILE:N	2.18	0.58
1:B:2125:ARG:NH1	1:B:2128:ARG:HD2	2.19	0.58
1:A:2085:ILE:HD12	1:A:2085:ILE:N	2.02	0.58
1:B:2050:LYS:HD2	1:B:2078:ARG:CZ	2.33	0.58
1:B:2180:LYS:NZ	1:B:2180:LYS:HB3	2.19	0.58
1:B:1730:CYS:C	1:B:1752:GLN:HG3	2.29	0.58
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.86	0.58
1:A:1786:ASN:HD21	1:B:1966:GLU:HG3	1.65	0.57
1:B:1925:HIS:HD2	4:B:5025:HOH:O	1.86	0.57
1:A:1848:GLU:HB2	4:A:5031:HOH:O	2.03	0.57
1:B:1541:GLU:HG3	1:B:1567:PHE:CE2	2.39	0.57
1:B:2010:ASP:OD1	1:B:2148:ARG:HG3	2.04	0.57
1:B:1917:ILE:HD12	1:B:1961:ARG:NH2	2.19	0.57
1:B:1711:ILE:HD12	1:B:1739:LEU:HD21	1.86	0.57
1:B:1922:GLN:CD	1:B:1954:ARG:HH12	2.12	0.57
1:B:2046:ARG:C	1:B:2047:LEU:HD12	2.29	0.57
1:B:2119:ARG:HG2	1:B:2119:ARG:HH11	1.68	0.57
1:A:2037:ARG:O	1:A:2040:LEU:N	2.37	0.57
1:B:1948:MSE:HE3	1:B:1950:LEU:HD21	1.87	0.57
1:A:1560:ASN:HD22	1:A:1560:ASN:N	1.93	0.57
1:A:2052:ARG:HG3	1:A:2052:ARG:NH1	2.20	0.57
1:A:2142:GLN:HB3	1:A:2190:LYS:HG3	1.87	0.57
1:B:2139:LEU:O	1:B:2140:SER:C	2.47	0.57
1:B:2147:SER:O	1:B:2148:ARG:C	2.48	0.56
1:A:1741:ARG:CZ	1:A:1744:GLN:HE22	2.18	0.56
1:A:1813:LYS:HB2	1:A:1813:LYS:NZ	2.19	0.56
1:A:2028:GLN:CD	1:A:2028:GLN:H	2.13	0.56
1:B:1786:ASN:OD1	1:B:1788:VAL:HG23	2.06	0.56
1:B:2148:ARG:O	1:B:2149:LEU:C	2.47	0.56
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.06	0.56
1:B:1527:SER:O	1:B:1530:VAL:HG22	2.06	0.56
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.56
1:A:2148:ARG:HH11	1:A:2148:ARG:HG2	1.71	0.56
1:B:1948:MSE:HE3	1:B:1950:LEU:HG	1.87	0.56
1:A:1903:ILE:HB	1:A:1915:THR:HG23	1.87	0.56
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.54	0.56
1:B:1657:TYR:HA	1:B:1690:ILE:HG12	1.87	0.56
1:A:2164:ASP:OD1	1:A:2167:ASP:HB2	2.06	0.56
1:B:1948:MSE:HE3	1:B:1950:LEU:CD2	2.36	0.56
1:B:2061:LYS:O	1:B:2061:LYS:HD3	2.06	0.56
1:B:2164:ASP:O	1:B:2166:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:ALA:H	1:B:2097:HIS:HE1	1.53	0.56
1:A:1667:LYS:C	1:A:1669:PHE:N	2.59	0.56
1:B:1730:CYS:CA	1:B:1752:GLN:HG3	2.36	0.56
1:B:1877:VAL:HG23	1:B:1928:SER:HB2	1.88	0.56
1:A:1776:GLN:O	1:B:1960:GLN:HG3	2.05	0.55
1:A:1980:ASP:O	1:A:1982:LYS:HD2	2.06	0.55
1:B:2082:LEU:N	1:B:2082:LEU:HD12	2.21	0.55
1:B:1940:ASN:HD21	1:B:1982:LYS:H	1.54	0.55
1:B:1955:GLY:HA2	1:B:1999:SER:HB3	1.88	0.55
1:A:2200:LYS:HA	1:A:2200:LYS:NZ	2.21	0.55
1:A:2140:SER:HB3	1:A:2151:LYS:HE2	1.88	0.55
1:B:1516:ARG:NH2	1:B:1534:ASP:HA	2.22	0.55
1:B:2132:GLU:O	1:B:2136:ILE:HG12	2.07	0.55
1:A:1860:LEU:HD23	1:A:2115:TRP:CZ3	2.41	0.55
1:B:1556:GLU:O	1:B:1558:GLY:N	2.38	0.55
1:B:1643:TRP:CE3	1:B:1649:PRO:HB3	2.41	0.55
1:A:2142:GLN:HG2	1:A:2190:LYS:HZ1	1.71	0.55
1:B:2148:ARG:NH2	1:B:2152:ILE:HD11	2.22	0.55
1:B:2148:ARG:CZ	1:B:2152:ILE:HD11	2.37	0.55
1:A:2142:GLN:HG2	1:A:2190:LYS:NZ	2.22	0.55
1:B:1560:ASN:H	1:B:1560:ASN:ND2	2.05	0.55
1:B:2100:SER:HA	1:B:2103:MSE:HE3	1.88	0.54
1:B:2139:LEU:O	1:B:2141:HIS:N	2.40	0.54
1:A:2034:LYS:HB2	1:B:1631:MSE:CE	2.32	0.54
1:B:1948:MSE:HE3	1:B:1950:LEU:CG	2.37	0.54
1:B:1593:ILE:HB	1:B:1625:SER:OG	2.08	0.54
1:B:1620:TYR:HB3	1:B:1726:THR:HB	1.88	0.54
1:B:1987:ILE:HB	1:B:2014:MSE:HG3	1.90	0.54
1:A:1968:LEU:HD21	1:B:1756:LEU:HD11	1.90	0.54
1:B:1829:ARG:NH2	1:B:2119:ARG:HE	2.06	0.54
1:B:2039:LYS:HB2	1:B:2039:LYS:HZ2	1.71	0.54
1:B:1505:THR:CB	1:B:1730:CYS:HB2	2.35	0.54
1:B:1922:GLN:HB2	1:B:1954:ARG:NH1	2.22	0.54
1:B:2037:ARG:NE	1:B:2083:LEU:HD11	2.21	0.54
1:A:2097:HIS:O	1:A:2102:ARG:HD3	2.08	0.54
1:B:2142:GLN:C	1:B:2142:GLN:CD	2.75	0.54
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.05	0.54
1:A:2050:LYS:NZ	1:A:2078:ARG:HD3	2.23	0.54
1:B:1654:GLN:O	1:B:1655:TYR:HB3	2.06	0.54
1:B:2037:ARG:HE	1:B:2083:LEU:HD11	1.72	0.54
1:B:2158:TRP:NE1	1:B:2185:LYS:HE3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.08	0.53
1:A:2196:GLN:HA	1:A:2196:GLN:NE2	2.22	0.53
1:B:1594:GLY:O	1:B:1624:ASN:HB2	2.08	0.53
1:A:1735:ILE:HD12	1:A:1735:ILE:N	2.22	0.53
1:A:1946:PRO:HG3	1:A:2130:LEU:HD21	1.90	0.53
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.05	0.53
1:B:2075:LEU:O	1:B:2079:GLU:HG3	2.09	0.53
1:B:1966:GLU:HG2	1:B:1969:LYS:CE	2.38	0.53
1:B:2131:ASN:ND2	1:B:2179:TYR:OH	2.42	0.53
1:A:2167:ASP:OD1	1:A:2170:GLN:HB2	2.09	0.52
1:B:1592:LYS:O	1:B:1593:ILE:HG13	2.08	0.52
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.08	0.52
1:B:1680:THR:HG22	1:B:1681:VAL:N	2.23	0.52
1:A:1655:TYR:CE1	1:A:1689:VAL:HG12	2.44	0.52
1:A:1860:LEU:HD23	1:A:2115:TRP:CH2	2.45	0.52
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.17	0.52
1:B:1783:MSE:SE	1:B:1786:ASN:HD21	2.42	0.52
1:A:2052:ARG:HG3	1:A:2052:ARG:HH11	1.73	0.52
1:B:1766:LEU:O	1:B:1767:GLY:C	2.52	0.52
1:B:1545:ASP:OD1	1:B:1549:GLU:N	2.42	0.52
1:A:1548:GLY:O	1:A:1606:LYS:HE2	2.09	0.52
1:A:1682:ILE:C	1:A:1684:GLY:N	2.68	0.52
1:A:1813:LYS:HB2	1:A:1813:LYS:HZ2	1.75	0.52
1:A:1820:ILE:HD12	1:A:1886:GLY:O	2.10	0.52
1:B:1537:PHE:CZ	1:B:1569:ILE:HD12	2.45	0.52
1:B:1952:ASN:OD1	1:B:1993:GLY:HA2	2.09	0.52
1:B:2082:LEU:N	1:B:2082:LEU:CD1	2.72	0.52
1:A:2124:TRP:CZ3	1:A:2169:ARG:HG3	2.45	0.52
1:B:2160:PRO:HD2	1:B:2163:VAL:HG21	1.90	0.52
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.44	0.52
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.56	0.52
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	1.91	0.52
1:A:1877:VAL:HG23	1:A:1931:LYS:HD3	1.91	0.52
1:A:2142:GLN:HB3	1:A:2190:LYS:HZ2	1.74	0.52
1:A:1508:VAL:HG21	1:A:1565:VAL:CG2	2.40	0.51
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.46	0.51
1:A:1655:TYR:CD1	1:A:1689:VAL:HG12	2.45	0.51
1:A:2127:ARG:NH2	1:A:2176:GLU:OE2	2.43	0.51
1:A:1673:ASN:OD1	1:A:1673:ASN:N	2.42	0.51
1:A:1846:MSE:HE2	1:A:2115:TRP:CH2	2.45	0.51
1:A:1881:ARG:HG2	1:A:1881:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1852:THR:C	1:B:1854:SER:H	2.18	0.51
1:A:2099:ARG:HG3	1:A:2099:ARG:NH1	2.26	0.51
1:B:2035:PHE:CE2	1:B:2039:LYS:HG2	2.45	0.51
1:B:2139:LEU:HD21	1:B:2154:ARG:NH1	2.25	0.51
1:A:1679:ARG:HG3	1:A:1679:ARG:NH1	2.25	0.51
1:A:2143:VAL:HG12	1:A:2144:GLY:N	2.25	0.51
1:B:1940:ASN:ND2	1:B:1982:LYS:H	2.08	0.51
1:B:1954:ARG:HG3	1:B:1954:ARG:NH1	2.24	0.51
1:B:2010:ASP:OD2	1:B:2148:ARG:HG3	2.08	0.51
1:B:1528:ALA:O	1:B:1530:VAL:N	2.44	0.51
1:B:1917:ILE:HD12	1:B:1961:ARG:HH22	1.74	0.51
1:B:1713:GLY:O	1:B:1717:ARG:HG3	2.11	0.51
1:A:1963:MSE:HE3	1:B:1783:MSE:HE2	1.93	0.51
1:A:1667:LYS:O	1:A:1669:PHE:N	2.43	0.51
1:A:1754:ILE:HD12	1:A:1783:MSE:HG2	1.92	0.51
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.91	0.51
1:B:2055:ARG:HG3	1:B:2055:ARG:NH1	2.25	0.51
1:B:2164:ASP:C	1:B:2166:GLU:N	2.68	0.51
1:A:1705:LEU:HB3	1:B:2000:TRP:CD1	2.46	0.51
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.91	0.51
1:A:2022:ALA:HB3	1:A:2103:MSE:HE2	1.92	0.51
1:A:2191:LEU:HD23	1:A:2191:LEU:O	2.11	0.51
1:A:2191:LEU:C	1:A:2191:LEU:CD2	2.83	0.51
1:A:1790:HIS:HB3	1:A:1869:THR:CG2	2.41	0.50
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.09	0.50
1:A:1785:ASN:N	1:A:1785:ASN:ND2	2.56	0.50
1:B:1682:ILE:C	1:B:1682:ILE:HD12	2.35	0.50
1:B:1856:PHE:CD2	1:B:1863:LYS:HE2	2.45	0.50
1:A:2131:ASN:HD22	1:A:2175:ILE:CG2	2.24	0.50
1:B:1785:ASN:N	1:B:1785:ASN:HD22	2.09	0.50
1:B:2119:ARG:HH11	1:B:2119:ARG:CG	2.24	0.50
1:B:1661:GLU:O	1:B:1664:GLU:N	2.44	0.50
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.12	0.50
1:B:1584:VAL:HG22	1:B:1619:ILE:HB	1.91	0.50
1:A:1682:ILE:CG1	1:A:1683:ASN:N	2.74	0.50
1:B:1772:THR:HG23	1:B:1776:GLN:HE22	1.76	0.50
1:B:1663:MSE:HB2	1:B:1688:PHE:CE1	2.47	0.50
1:A:2085:ILE:O	1:A:2088:GLN:HB2	2.12	0.50
1:A:2102:ARG:HH11	1:B:1694:ILE:HG23	1.76	0.50
1:A:2167:ASP:HB3	1:A:2170:GLN:HB2	1.94	0.50
1:B:1671:LYS:C	1:B:1673:ASN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1936:ILE:HG12	1:B:1947:MSE:SE	2.61	0.50
1:A:1778:GLY:HA2	1:A:1783:MSE:HE2	1.93	0.50
1:A:2021:ARG:HE	1:A:2095:ASP:CG	2.20	0.50
1:A:2192:GLU:O	1:A:2196:GLN:HB2	2.11	0.49
1:B:2188:GLY:C	1:B:2189:LEU:HD23	2.36	0.49
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.59	0.49
1:A:1737:ALA:O	1:A:1740:VAL:CG1	2.60	0.49
1:B:1513:GLU:O	1:B:1517:GLN:HG3	2.11	0.49
1:B:1660:SER:HA	1:B:1688:PHE:HE1	1.77	0.49
1:B:1730:CYS:O	1:B:1731:ARG:HB3	2.13	0.49
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.12	0.49
1:A:1837:ASN:OD1	1:A:1992:THR:HG22	2.12	0.49
1:A:2017:ASP:OD2	1:A:2115:TRP:HB2	2.12	0.49
1:A:2097:HIS:CE1	1:B:1632:ALA:H	2.30	0.49
1:A:2193:SER:O	1:A:2195:ALA:N	2.46	0.49
1:A:1497:ARG:HD3	1:A:1510:ASP:OD2	2.12	0.49
1:B:1711:ILE:HD11	1:B:1735:ILE:HG12	1.95	0.49
1:B:1747:ILE:N	1:B:1747:ILE:HD12	2.27	0.49
1:B:1966:GLU:HG2	1:B:1969:LYS:HD2	1.94	0.49
1:A:1682:ILE:HG23	1:A:1687:ARG:HG3	1.94	0.49
1:A:1768:ARG:HD2	1:A:1770:VAL:HG22	1.94	0.49
1:A:2058:LEU:HD22	1:A:2068:HIS:CE1	2.46	0.49
1:B:1836:THR:HG22	1:B:1838:ASP:N	2.26	0.49
1:A:1494:GLN:OE1	1:A:1496:LYS:HG2	2.13	0.49
1:A:2041:LEU:HD12	1:A:2044:MSE:CE	2.42	0.49
1:A:2066:GLU:H	1:A:2066:GLU:CD	2.21	0.49
1:B:1772:THR:HG23	1:B:1776:GLN:NE2	2.27	0.49
1:A:1744:GLN:NE2	1:A:1744:GLN:HA	2.28	0.49
1:B:2160:PRO:HD2	1:B:2163:VAL:CG2	2.43	0.49
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.77	0.49
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.94	0.49
1:A:2125:ARG:HH12	1:A:2128:ARG:HH21	1.61	0.49
1:A:2198:LEU:C	1:A:2198:LEU:HD23	2.37	0.49
1:B:1748:GLN:O	1:B:1792:THR:HA	2.13	0.49
1:B:1495:PRO:HG2	1:B:1496:LYS:H	1.78	0.48
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.13	0.48
1:A:1803:ILE:HG22	1:A:1807:MSE:CE	2.44	0.48
1:A:1629:ILE:HG12	2:A:3203:ACO:C6A	2.43	0.48
1:A:1963:MSE:HE1	1:B:1755:ILE:HA	1.94	0.48
1:A:1968:LEU:HD12	1:B:1783:MSE:HE1	1.96	0.48
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.13	0.48
1:A:1841:TYR:CZ	1:A:1896:THR:HG21	2.48	0.48
1:A:2144:GLY:O	1:A:2145:GLU:C	2.55	0.48
1:B:1676:LEU:HD12	1:B:1692:THR:HG21	1.95	0.48
1:B:1682:ILE:HG13	1:B:1685:GLU:O	2.14	0.48
1:B:1975:VAL:O	1:B:1979:VAL:HG23	2.12	0.48
1:A:1735:ILE:H	1:A:1735:ILE:CD1	2.22	0.48
1:A:2156:ARG:HG2	1:A:2159:TYR:CE1	2.49	0.48
1:B:1600:GLU:OE1	1:B:1600:GLU:N	2.45	0.48
1:A:2083:LEU:HD12	1:A:2083:LEU:HA	1.72	0.48
1:A:1748:GLN:O	1:A:1792:THR:HA	2.13	0.48
1:A:1508:VAL:HG21	1:A:1565:VAL:HG21	1.96	0.48
1:A:1651:LYS:O	1:A:1651:LYS:HG3	2.14	0.48
1:A:2138:ARG:C	1:A:2140:SER:H	2.22	0.48
1:B:1625:SER:OG	1:B:1731:ARG:NH2	2.45	0.48
1:B:1645:ASP:O	1:B:1647:ALA:O	2.32	0.47
1:A:1484:ALA:O	1:A:1485:THR:O	2.32	0.47
1:A:1720:HIS:HD2	1:A:1941:ASN:ND2	2.13	0.47
1:A:1842:ASP:HA	1:A:1897:ARG:HH11	1.79	0.47
1:A:2082:LEU:HA	1:A:2085:ILE:HD13	1.96	0.47
1:B:2058:LEU:HD21	1:B:2071:ILE:HB	1.96	0.47
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.62	0.47
1:A:1909:ASN:HB3	1:A:1912:SER:HB2	1.96	0.47
1:B:1966:GLU:HG2	1:B:1969:LYS:CD	2.44	0.47
1:B:2138:ARG:HG3	1:B:2138:ARG:HH11	1.79	0.47
1:B:1985:ILE:HD12	1:B:2012:MSE:HG2	1.96	0.47
1:A:1522:GLN:NE2	1:A:1574:PRO:HD2	2.30	0.47
1:A:1689:VAL:HG23	1:A:1691:LYS:HE2	1.97	0.47
1:A:2197:ASP:O	1:A:2201:LYS:HB3	2.15	0.47
1:B:1598:PRO:HG2	1:B:1698:ASP:OD1	2.15	0.47
1:B:1786:ASN:OD1	1:B:1786:ASN:C	2.57	0.47
1:A:1508:VAL:CG2	1:A:1565:VAL:HG21	2.44	0.47
1:A:1842:ASP:OD1	1:A:1844:ARG:NH1	2.43	0.47
1:B:1583:VAL:HG22	1:B:1584:VAL:N	2.29	0.47
1:B:2082:LEU:O	1:B:2083:LEU:C	2.58	0.47
1:A:1667:LYS:NZ	1:A:1670:ASP:HA	2.29	0.47
1:A:2128:ARG:HD3	1:A:2171:VAL:HG11	1.97	0.47
1:A:2138:ARG:HB3	1:A:2138:ARG:NH1	2.29	0.47
1:B:1765:MSE:C	1:B:1766:LEU:HD12	2.39	0.47
1:B:1797:LEU:O	1:B:1801:GLU:HG3	2.15	0.47
1:B:2180:LYS:HB3	1:B:2180:LYS:HZ2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2041:LEU:HA	1:B:2044:MSE:HG3	1.97	0.47
1:A:2002:VAL:HG23	1:A:2003:VAL:HG13	1.97	0.46
1:B:1523:TRP:HB3	1:B:1530:VAL:HG21	1.98	0.46
1:B:1810:VAL:HG23	1:B:1811:PRO:CD	2.45	0.46
1:B:2078:ARG:CZ	1:B:2082:LEU:HD11	2.45	0.46
1:A:1881:ARG:HG2	1:A:1881:ARG:NH1	2.31	0.46
1:B:1940:ASN:ND2	1:B:1983:GLN:NE2	2.50	0.46
1:B:2064:ALA:HB3	1:B:2067:VAL:CG2	2.45	0.46
1:A:1659:THR:O	1:A:1660:SER:C	2.57	0.46
1:A:1681:VAL:HA	1:A:1685:GLU:O	2.15	0.46
1:A:1686:GLU:C	1:A:1687:ARG:HG2	2.40	0.46
1:A:2143:VAL:O	1:A:2145:GLU:N	2.49	0.46
1:B:1499:LYS:HB2	1:B:1499:LYS:NZ	2.31	0.46
1:B:2139:LEU:HD11	1:B:2154:ARG:HH11	1.81	0.46
1:B:1917:ILE:O	1:B:1917:ILE:HG12	2.14	0.46
1:B:1514:LEU:HD22	1:B:1797:LEU:HD13	1.97	0.46
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	2.16	0.46
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.79	0.46
1:A:1657:TYR:HB2	1:A:1688:PHE:O	2.16	0.46
1:A:1963:MSE:CE	1:B:1755:ILE:HA	2.46	0.46
1:B:1671:LYS:C	1:B:1673:ASN:N	2.74	0.46
1:B:1906:ASP:H	1:B:1912:SER:HB2	1.80	0.46
1:A:1526:PHE:CD1	1:A:1526:PHE:C	2.94	0.45
1:A:1730:CYS:O	1:A:1731:ARG:HB3	2.16	0.45
1:A:2102:ARG:NH2	1:B:1700:LEU:HB2	2.31	0.45
1:A:2110:SER:O	1:A:2111:LYS:HG3	2.16	0.45
1:A:2196:GLN:NE2	1:A:2196:GLN:CA	2.77	0.45
1:B:1733:VAL:HG22	1:B:1755:ILE:CD1	2.44	0.45
1:B:1906:ASP:H	1:B:1912:SER:CB	2.29	0.45
1:A:1575:GLU:HG2	1:A:1576:TYR:CD1	2.51	0.45
1:A:2037:ARG:HH11	1:A:2037:ARG:CB	2.20	0.45
1:A:2148:ARG:HG2	1:A:2148:ARG:NH1	2.32	0.45
1:B:1901:ASN:HB3	1:B:1917:ILE:HG23	1.99	0.45
1:A:1619:ILE:HD12	1:A:1725:ILE:CG2	2.45	0.45
1:B:1985:ILE:HD12	1:B:2012:MSE:CG	2.47	0.45
1:A:1618:ARG:HE	1:A:1618:ARG:C	2.24	0.45
1:A:1903:ILE:N	1:A:1903:ILE:HD12	2.32	0.45
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.99	0.45
1:B:2144:GLY:O	1:B:2145:GLU:C	2.59	0.45
1:A:1588:ASP:OD1	1:A:1590:THR:OG1	2.35	0.45
1:A:2030:MSE:HG3	1:B:1631:MSE:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2129:ARG:HG3	1:A:2129:ARG:HH11	1.82	0.45
1:B:1902:LEU:HD21	1:B:1914:GLU:CD	2.42	0.45
1:B:2044:MSE:HE3	1:B:2044:MSE:HB3	1.84	0.45
1:B:2126:LEU:HD22	1:B:2130:LEU:HD13	1.99	0.45
1:A:1720:HIS:HD2	1:A:1941:ASN:HD21	1.63	0.45
1:A:1901:ASN:O	1:A:1916:LEU:HD12	2.16	0.45
1:A:2167:ASP:CG	1:A:2170:GLN:HB2	2.42	0.45
1:B:2187:LYS:C	1:B:2189:LEU:H	2.24	0.45
1:A:1610:TYR:CE1	1:A:1614:ARG:CZ	3.00	0.45
1:A:1612:ARG:O	1:A:1814:ARG:NH2	2.37	0.45
1:A:1991:PRO:C	1:A:1993:GLY:H	2.25	0.45
1:B:1643:TRP:CD1	1:B:1643:TRP:H	2.35	0.45
1:A:1667:LYS:O	1:A:1667:LYS:HD3	2.17	0.45
1:A:1667:LYS:HZ1	1:A:1672:GLU:CD	2.24	0.45
1:A:1784:TYR:CD1	1:A:1792:THR:HG23	2.51	0.45
1:A:1956:PHE:HB2	1:B:1756:LEU:HD23	1.99	0.44
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.77	0.44
1:B:1951:ALA:O	1:B:1990:PRO:HD2	2.18	0.44
1:A:1734:GLY:C	1:A:1736:GLY:N	2.74	0.44
1:B:1661:GLU:O	1:B:1662:GLY:C	2.60	0.44
1:B:1744:GLN:O	1:B:1790:HIS:CE1	2.70	0.44
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.98	0.44
1:B:2027:PRO:O	1:B:2028:GLN:C	2.60	0.44
1:A:1708:SER:OG	1:A:1735:ILE:HG12	2.18	0.44
1:A:1803:ILE:HG22	1:A:1807:MSE:HE2	2.00	0.44
1:A:1545:ASP:OD2	1:A:1545:ASP:C	2.61	0.44
1:A:1991:PRO:O	1:A:2019:ASN:O	2.34	0.44
1:A:1996:ARG:NE	1:A:2026:GLU:HG2	2.32	0.44
1:B:1657:TYR:HB2	1:B:1688:PHE:O	2.18	0.44
1:B:2126:LEU:CD2	1:B:2130:LEU:HD13	2.48	0.44
1:B:1818:VAL:O	1:B:1820:ILE:HD12	2.17	0.44
1:A:1713:GLY:O	1:A:1717:ARG:HG3	2.18	0.44
1:B:1877:VAL:HG12	1:B:1878:VAL:N	2.33	0.44
1:A:2000:TRP:CD1	1:B:1705:LEU:HB3	2.53	0.44
1:B:1496:LYS:HB3	1:B:1507:TYR:CE2	2.53	0.44
1:B:1532:LEU:HD13	1:B:1536:PHE:CE1	2.52	0.44
1:B:2082:LEU:HB3	1:B:2086:TYR:CD1	2.53	0.44
1:B:1657:TYR:CD2	1:B:1687:ARG:CB	2.99	0.44
1:B:1783:MSE:HA	1:B:1786:ASN:ND2	2.33	0.44
1:B:1640:GLN:O	1:B:1656:LEU:HA	2.17	0.43
1:B:1669:PHE:N	1:B:1669:PHE:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2047:LEU:HD12	1:B:2047:LEU:N	2.32	0.43
1:A:1735:ILE:O	1:A:1739:LEU:HG	2.18	0.43
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.96	0.43
1:A:2072:SER:O	1:A:2075:LEU:HB3	2.18	0.43
1:B:1594:GLY:O	1:B:1624:ASN:CB	2.66	0.43
1:B:1645:ASP:CG	1:B:1647:ALA:O	2.61	0.43
1:B:1844:ARG:HG3	1:B:1844:ARG:HH11	1.82	0.43
1:B:2100:SER:CA	1:B:2103:MSE:HE3	2.48	0.43
1:A:1852:THR:C	1:A:1854:SER:H	2.26	0.43
1:B:1607:VAL:O	1:B:1610:TYR:HB3	2.17	0.43
1:B:2070:GLN:HG3	1:B:2074:GLN:NE2	2.33	0.43
1:B:1602:GLU:O	1:B:1606:LYS:HB2	2.18	0.43
1:B:1644:ASN:OD1	1:B:1651:LYS:O	2.37	0.43
1:A:1903:ILE:HA	1:A:1904:PRO:HD3	1.86	0.43
1:A:2153:ALA:O	1:A:2154:ARG:C	2.62	0.43
1:B:1676:LEU:HD12	1:B:1692:THR:CG2	2.48	0.43
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.48	0.43
1:A:2128:ARG:HD2	1:A:2128:ARG:C	2.44	0.43
1:B:1827:TRP:CD2	1:B:1828:ASP:N	2.87	0.43
1:B:1829:ARG:CZ	1:B:2119:ARG:NE	2.74	0.43
1:A:1895:GLU:HA	1:A:1895:GLU:OE2	2.18	0.43
1:A:1990:PRO:HB2	1:A:1991:PRO:HD2	2.01	0.43
1:A:2197:ASP:O	1:A:2200:LYS:O	2.36	0.43
1:B:1644:ASN:ND2	1:B:1654:GLN:HE21	2.03	0.43
1:B:1895:GLU:OE2	1:B:1897:ARG:NH2	2.35	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.19	0.43
1:A:1735:ILE:HG23	1:B:2001:VAL:HG21	2.00	0.43
1:A:2165:HIS:ND1	1:A:2165:HIS:N	2.65	0.43
1:B:1881:ARG:HG3	1:B:1881:ARG:HH11	1.83	0.43
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.82	0.43
1:B:1617:PRO:HG2	1:B:1807:MSE:HE3	2.00	0.43
1:B:1865:SER:O	1:B:1882:ALA:HA	2.18	0.43
1:A:1702:VAL:HA	1:A:1705:LEU:HD22	2.01	0.43
1:A:1825:ASP:OD1	1:A:1825:ASP:C	2.60	0.43
1:B:1660:SER:HA	1:B:1688:PHE:CE1	2.53	0.43
1:A:1604:PHE:CD2	1:A:1604:PHE:C	2.97	0.42
1:A:1747:ILE:HD12	1:A:1803:ILE:HG13	2.02	0.42
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.19	0.42
1:B:1541:GLU:HA	1:B:1567:PHE:HD2	1.84	0.42
1:B:1592:LYS:C	1:B:1593:ILE:CG1	2.92	0.42
1:B:1728:VAL:HG12	1:B:1752:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1783:MSE:HB3	1:A:1789:SER:OG	2.20	0.42
1:A:1841:TYR:CD1	1:A:1841:TYR:C	2.98	0.42
1:A:2154:ARG:O	1:A:2157:SER:OG	2.38	0.42
1:B:2070:GLN:OE1	1:B:2070:GLN:HA	2.19	0.42
1:A:1702:VAL:HA	1:A:1705:LEU:HB2	2.00	0.42
1:B:1836:THR:O	1:B:1837:ASN:C	2.63	0.42
1:B:1681:VAL:O	1:B:1681:VAL:HG22	2.20	0.42
1:A:2052:ARG:HH11	1:A:2052:ARG:CG	2.32	0.42
1:B:2179:TYR:O	1:B:2183:ASP:HB2	2.20	0.42
1:B:1644:ASN:HD21	1:B:1654:GLN:NE2	2.05	0.42
1:B:1836:THR:O	1:B:1838:ASP:N	2.52	0.42
1:B:2083:LEU:HD23	1:B:2083:LEU:HA	1.90	0.42
1:A:2037:ARG:O	1:A:2038:GLU:C	2.63	0.42
1:A:2108:VAL:HG11	1:B:1702:VAL:HG23	2.01	0.42
1:B:1668:LYS:C	1:B:1670:ASP:H	2.28	0.41
1:A:1638:LEU:CD1	1:A:1658:LEU:HD22	2.50	0.41
1:A:1819:PRO:O	1:A:1888:PRO:HG3	2.20	0.41
1:A:1901:ASN:ND2	1:A:1903:ILE:HD11	2.35	0.41
1:A:1952:ASN:HA	1:A:1994:GLU:O	2.20	0.41
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.55	0.41
1:B:1495:PRO:O	1:B:1496:LYS:C	2.63	0.41
1:B:1831:VAL:HG22	1:B:2119:ARG:HB2	2.02	0.41
1:B:1702:VAL:HA	1:B:1705:LEU:HD12	2.01	0.41
1:B:1766:LEU:N	1:B:1766:LEU:CD1	2.84	0.41
1:B:1813:LYS:HG3	1:B:1816:MSE:HG2	2.02	0.41
1:B:1881:ARG:HG3	1:B:1881:ARG:NH1	2.36	0.41
1:B:1998:GLY:O	1:B:2001:VAL:CG1	2.68	0.41
1:B:2148:ARG:NE	1:B:2152:ILE:HD11	2.36	0.41
1:A:1737:ALA:O	1:A:1740:VAL:HG13	2.20	0.41
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.20	0.41
1:A:1800:VAL:O	1:A:1804:VAL:HG23	2.20	0.41
1:A:1680:THR:CG2	1:A:1681:VAL:N	2.82	0.41
1:A:1680:THR:HB	1:A:1687:ARG:O	2.21	0.41
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.56	0.41
1:A:1643:TRP:CH2	1:A:1649:PRO:HB3	2.55	0.41
1:A:1686:GLU:O	1:A:1687:ARG:HG2	2.21	0.41
1:A:2078:ARG:HA	1:A:2081:GLU:HG2	2.02	0.41
1:B:1702:VAL:HG23	1:B:1703:GLU:N	2.36	0.41
1:A:1836:THR:O	1:A:1838:ASP:N	2.46	0.41
1:B:1834:THR:HA	1:B:1835:PRO:HD3	1.83	0.41
1:B:1842:ASP:OD1	1:B:1844:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2022:ALA:O	1:A:2098:ASP:HA	2.21	0.41
1:A:2102:ARG:NH1	1:B:1694:ILE:HG23	2.36	0.41
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.03	0.41
1:A:2118:ALA:O	1:A:2119:ARG:C	2.63	0.41
1:B:1615:GLY:HA2	1:B:1814:ARG:NH1	2.36	0.41
1:B:1619:ILE:HD12	1:B:1619:ILE:N	2.36	0.41
1:B:1645:ASP:C	1:B:1647:ALA:N	2.78	0.41
1:B:1755:ILE:N	1:B:1755:ILE:CD1	2.83	0.41
1:B:1968:LEU:HB2	4:B:5028:HOH:O	2.20	0.41
1:B:2026:GLU:O	1:B:2027:PRO:C	2.63	0.41
1:A:1783:MSE:HG3	1:A:1788:VAL:HB	2.02	0.41
1:A:1832:ASP:HB2	1:A:1858:TYR:N	2.35	0.40
1:B:1852:THR:C	1:B:1854:SER:N	2.79	0.40
1:B:1852:THR:O	1:B:1854:SER:N	2.49	0.40
1:B:2061:LYS:O	1:B:2062:SER:HB3	2.21	0.40
1:B:2091:LEU:HD12	1:B:2091:LEU:HA	1.90	0.40
1:B:2136:ILE:HD13	1:B:2155:ILE:HD12	2.03	0.40
1:B:2140:SER:O	1:B:2142:GLN:N	2.54	0.40
1:A:1869:THR:HG22	1:A:1870:LEU:N	2.36	0.40
1:A:1968:LEU:HD12	1:B:1783:MSE:CE	2.52	0.40
1:A:2056:SER:O	1:A:2060:ASN:N	2.54	0.40
1:A:2125:ARG:HH12	1:A:2128:ARG:NH2	2.20	0.40
1:B:1668:LYS:HD3	1:B:1668:LYS:HA	1.91	0.40
1:B:1728:VAL:O	1:B:1749:VAL:HG23	2.21	0.40
1:A:1803:ILE:CG2	1:A:1807:MSE:HE2	2.51	0.40
1:A:1530:VAL:O	1:A:1530:VAL:HG23	2.20	0.40
1:B:1545:ASP:O	1:B:1548:GLY:N	2.45	0.40
1:B:1593:ILE:O	1:B:1594:GLY:C	2.64	0.40
1:B:1816:MSE:O	1:B:1817:PRO:C	2.63	0.40
1:B:2052:ARG:HG2	1:B:2052:ARG:HH11	1.87	0.40
1:B:2178:ASN:HD22	1:B:2181:THR:CB	2.34	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	718/805 (89%)	640 (89%)	61 (8%)	17 (2%)	4	12
1	B	694/805 (86%)	608 (88%)	61 (9%)	25 (4%)	2	6
All	All	1412/1610 (88%)	1248 (88%)	122 (9%)	42 (3%)	3	8

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	A	1991	PRO
1	A	2144	GLY
1	A	2194	PHE
1	B	1838	ASP
1	B	1991	PRO
1	B	1992	THR
1	A	1679	ARG
1	A	1997	GLY
1	A	2142	GLN
1	B	1529	ASP
1	B	1683	ASN
1	B	1684	GLY
1	B	2140	SER
1	B	2141	HIS
1	B	2143	VAL
1	B	2165	HIS
1	A	1485	THR
1	A	1668	LYS
1	A	1744	GLN
1	B	1526	PHE
1	B	2061	LYS
1	B	2084	PRO
1	B	2148	ARG
1	A	1527	SER
1	A	1826	THR
1	A	2161	ALA
1	B	1558	GLY
1	B	1837	ASN
1	A	1731	ARG
1	A	2139	LEU
1	B	1731	ARG
1	B	1853	GLU

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Mol	Chain	Res	Type
1	A	1682	ILE
1	B	1508	VAL
1	B	1534	ASP
1	B	2038	GLU
1	B	2145	GLU
1	A	2143	VAL
1	B	1843	VAL
1	B	2144	GLY
1	B	1557	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/668 (92%)	554 (90%)	58 (10%)	8	20
1	B	591/668 (88%)	538 (91%)	53 (9%)	9	23
All	All	1203/1336 (90%)	1092 (91%)	111 (9%)	8	22

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1514	LEU
1	A	1532	LEU
1	A	1541	GLU
1	A	1554	GLU
1	A	1560	ASN
1	A	1570	THR
1	A	1580	ARG
1	A	1589	ILE
1	A	1602	GLU
1	A	1618	ARG
1	A	1634	GLU
1	A	1650	ASP
1	A	1667	LYS
1	A	1668	LYS

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Mol	Chain	Res	Type
1	A	1673	ASN
1	A	1675	VAL
1	A	1680	THR
1	A	1682	ILE
1	A	1697	GLU
1	A	1705	LEU
1	A	1706	ARG
1	A	1733	VAL
1	A	1735	ILE
1	A	1740	VAL
1	A	1757	THR
1	A	1772	THR
1	A	1780	THR
1	A	1781	GLN
1	A	1783	MSE
1	A	1785	ASN
1	A	1786	ASN
1	A	1813	LYS
1	A	1820	ILE
1	A	1821	LEU
1	A	1823	THR
1	A	1860	LEU
1	A	1877	VAL
1	A	1879	VAL
1	A	1884	LEU
1	A	1895	GLU
1	A	1991	PRO
1	A	1999	SER
1	A	2001	VAL
1	A	2028	GLN
1	A	2037	ARG
1	A	2038	GLU
1	A	2085	ILE
1	A	2126	LEU
1	A	2138	ARG
1	A	2145	GLU
1	A	2163	VAL
1	A	2181	THR
1	A	2183	ASP
1	A	2190	LYS
1	A	2192	GLU
1	A	2196	GLN

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Mol	Chain	Res	Type
1	A	2200	LYS
1	A	2201	LYS
1	B	1499	LYS
1	B	1513	GLU
1	B	1527	SER
1	B	1534	ASP
1	B	1540	ASN
1	B	1553	VAL
1	B	1555	ARG
1	B	1560	ASN
1	B	1568	LYS
1	B	1575	GLU
1	B	1602	GLU
1	B	1618	ARG
1	B	1621	LEU
1	B	1638	LEU
1	B	1675	VAL
1	B	1726	THR
1	B	1739	LEU
1	B	1755	ILE
1	B	1757	THR
1	B	1768	ARG
1	B	1772	THR
1	B	1781	GLN
1	B	1810	VAL
1	B	1839	GLU
1	B	1857	GLU
1	B	1891	VAL
1	B	1902	LEU
1	B	1910	PRO
1	B	1917	ILE
1	B	1923	VAL
1	B	1980	ASP
1	B	1991	PRO
1	B	2001	VAL
1	B	2024	VAL
1	B	2026	GLU
1	B	2027	PRO
1	B	2037	ARG
1	B	2039	LYS
1	B	2040	LEU
1	B	2044	MSE

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Mol	Chain	Res	Type
1	B	2055	ARG
1	B	2061	LYS
1	B	2063	LEU
1	B	2066	GLU
1	B	2088	GLN
1	B	2091	LEU
1	B	2092	GLN
1	B	2126	LEU
1	B	2130	LEU
1	B	2142	GLN
1	B	2145	GLU
1	B	2166	GLU
1	B	2182	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1501	HIS
1	A	1522	GLN
1	A	1560	ASN
1	A	1599	GLN
1	A	1624	ASN
1	A	1640	GLN
1	A	1654	GLN
1	A	1720	HIS
1	A	1744	GLN
1	A	1785	ASN
1	A	1786	ASN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1934	GLN
1	A	1941	ASN
1	A	2008	ASN
1	A	2011	GLN
1	A	2045	ASN
1	A	2060	ASN
1	A	2068	HIS
1	A	2097	HIS
1	A	2131	ASN
1	A	2178	ASN
1	A	2196	GLN

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Mol	Chain	Res	Type
1	B	1525	ASN
1	B	1540	ASN
1	B	1560	ASN
1	B	1581	GLN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1654	GLN
1	B	1744	GLN
1	B	1748	GLN
1	B	1776	GLN
1	B	1785	ASN
1	B	1925	HIS
1	B	1934	GLN
1	B	1940	ASN
1	B	2057	GLN
1	B	2074	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2141	HIS
1	B	2178	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
3	ADE	B	3190	-	11,11,11	1.57	2 (18%)	15,15,15	0.65	0
2	ACO	A	3203	-	47,50,53	1.19	5 (10%)	69,75,79	1.47	8 (11%)

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	ADE	B	3190	-	-	-	0/2/2/2
2	ACO	A	3203	-	-	9/48/64/67	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3203	ACO	P2A-O3A	-3.36	1.55	1.59
2	A	3203	ACO	C4A-N3A	2.76	1.39	1.34
3	B	3190	ADE	C4-N3	2.43	1.38	1.35
3	B	3190	ADE	C8-N7	2.21	1.36	1.32
2	A	3203	ACO	CDP-CBP	2.11	1.58	1.53
2	A	3203	ACO	C5A-C6A	2.04	1.46	1.41
2	A	3203	ACO	O6A-CCP	2.02	1.50	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3203	ACO	C3P-N4P-C5P	5.52	133.10	122.82
2	A	3203	ACO	O6A-CCP-CBP	5.46	119.33	110.55
2	A	3203	ACO	C2P-C3P-N4P	-3.38	104.64	112.31
2	A	3203	ACO	O3A-P2A-O4A	-2.58	102.96	110.70
2	A	3203	ACO	C4B-O4B-C1B	2.14	114.20	109.47
2	A	3203	ACO	CEP-CBP-CAP	2.14	112.41	108.77
2	A	3203	ACO	O2B-C2B-C3B	2.11	117.09	111.19
2	A	3203	ACO	C2A-N1A-C6A	2.04	122.08	118.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

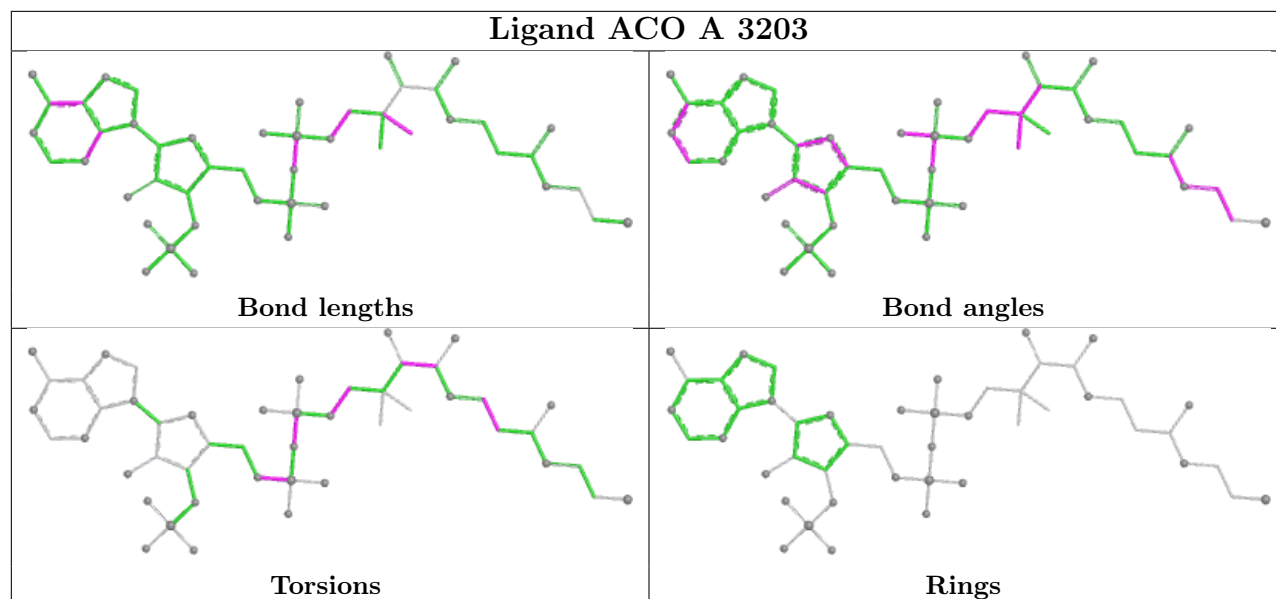
Mol	Chain	Res	Type	Atoms
2	A	3203	ACO	C5B-O5B-P1A-O1A
2	A	3203	ACO	C5B-O5B-P1A-O2A
2	A	3203	ACO	C5B-O5B-P1A-O3A
2	A	3203	ACO	CBP-CCP-O6A-P2A
2	A	3203	ACO	N8P-C9P-CAP-CBP
2	A	3203	ACO	P1A-O3A-P2A-O5A
2	A	3203	ACO	C5P-C6P-C7P-N8P
2	A	3203	ACO	O9P-C9P-CAP-CBP
2	A	3203	ACO	P1A-O3A-P2A-O4A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3203	ACO	4	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	703/805 (87%)	0.10	18 (2%) 57 54	22, 37, 58, 74	0
1	B	679/805 (84%)	0.09	17 (2%) 58 55	20, 38, 59, 69	0
All	All	1382/1610 (85%)	0.10	35 (2%) 58 55	20, 38, 59, 74	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2143	VAL	6.0
1	A	2202	ILE	4.1
1	A	1484	ALA	3.9
1	A	2194	PHE	3.7
1	B	1495	PRO	3.7
1	B	1527	SER	3.6
1	A	1681	VAL	3.5
1	A	1685	GLU	3.4
1	A	1684	GLY	3.1
1	A	2203	ARG	3.1
1	B	1528	ALA	3.0
1	A	2143	VAL	3.0
1	B	1851	GLU	3.0
1	B	1682	ILE	2.9
1	A	2076	ALA	2.8
1	A	2199	ALA	2.8
1	A	2201	LYS	2.7
1	A	2145	GLU	2.7
1	A	2179	TYR	2.7
1	B	2141	HIS	2.7
1	B	2144	GLY	2.6
1	B	1681	VAL	2.6
1	A	1680	THR	2.5
1	B	1697	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	2080	ARG	2.4
1	B	1680	THR	2.4
1	B	1839	GLU	2.3
1	B	1683	ASN	2.3
1	A	1667	LYS	2.3
1	B	2142	GLN	2.3
1	A	2198	LEU	2.3
1	A	2196	GLN	2.3
1	B	1557	PRO	2.2
1	A	1855	GLY	2.1
1	B	1497	ARG	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](#)

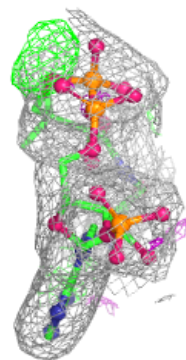
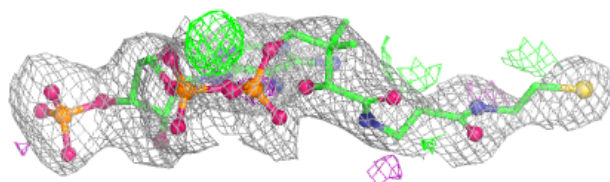
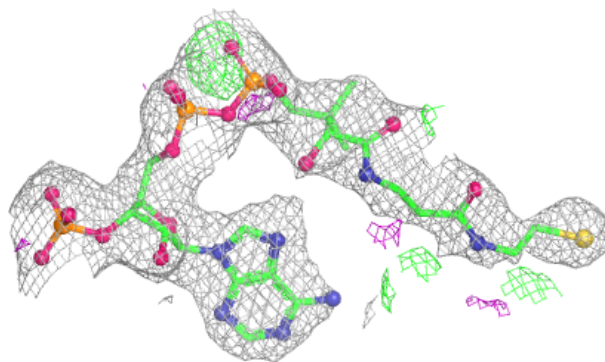
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ADE	B	3190	10/10	0.74	0.18	61,63,63,64	0
2	ACO	A	3203	48/51	0.87	0.12	56,68,77,79	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 ACO A 3203:

$2mF_o - DF_c$ (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.