



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 02:15 AM EDT

PDB ID : 3PGQ
Title : Crystal Structure of the Carboxyltransferase Domain of *S. cerevisiae* Acetyl CoA Carboxylase in Complex with Pinoxaden
Authors : Tong, L.; Yu, L.P.C.; Kim, Y.S.
Deposited on : 2010-11-02
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

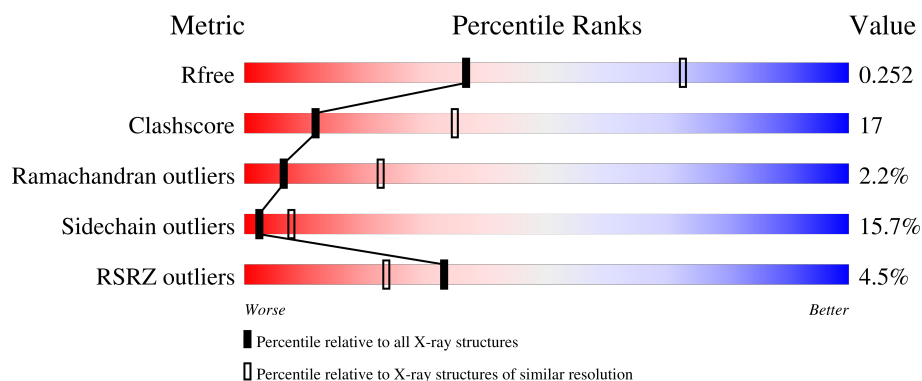
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	764	<div> <div>3%</div> <div>59% 24% 6% 10%</div> </div>
1	B	764	<div> <div>5%</div> <div>56% 25% 7% 11%</div> </div>
1	C	764	<div> <div>4%</div> <div>58% 25% 5% 12%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GY3	B	2240	-	-	X	-

2 Entry composition [i](#)

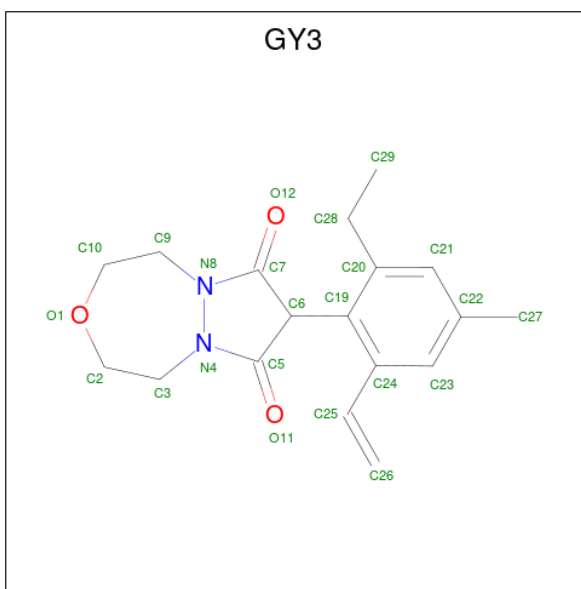
There are 2 unique types of molecules in this entry. The entry contains 16368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

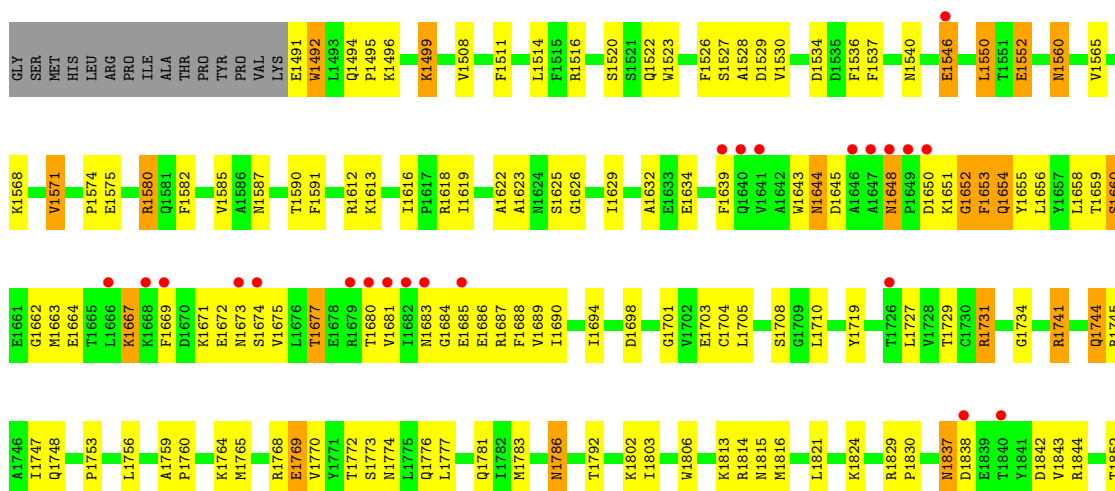
- Molecule 1 is a protein called Acetyl-CoA carboxylase.

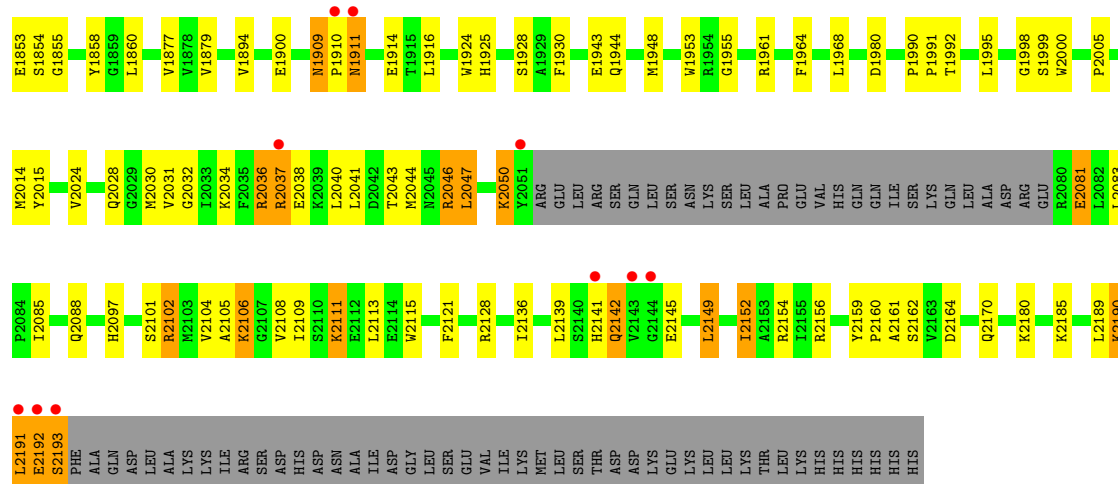
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	688	Total	C	N	O	S	0	0	0
			5491	3500	944	1028	19			
1	B	680	Total	C	N	O	S	0	0	0
			5421	3456	932	1014	19			
1	C	675	Total	C	N	O	S	0	0	0
			5387	3428	927	1013	19			

- Molecule 2 is 8-(2-ethenyl-6-ethyl-4-methylphenyl)tetrahydro-7H-pyrazolo[1,2-d][1,4,5]oxadiazepine-7,9(8H)-dione (three-letter code: GY3) (formula: C₁₈H₂₂N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	18	2	3		
2	B	1	Total	C	N	O	0	0
			23	18	2	3		
2	B	1	Total	C	N	O	0	0
			23	18	2	3		





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.18Å 123.42Å 145.71Å 90.00° 94.29° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.80) 98.4 (29.93-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.197 , 0.239 0.221 , 0.252	Depositor DCC
R_{free} test set	5269 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16368	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: GY3

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	0.62	0/5614	0.66	0/7605
1	B	0.61	0/5542	0.70	7/7509 (0.1%)
1	C	0.60	0/5505	0.65	1/7454 (0.0%)
All	All	0.61	0/16661	0.67	8/22568 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	1
All	All	0	7

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1481	ARG	O-C-N	-13.54	95.38	121.10
1	B	1481	ARG	CB-CA-C	10.40	131.20	110.40
1	B	1481	ARG	C-N-CD	-9.78	99.09	120.60
1	B	1481	ARG	CA-C-N	9.54	143.81	117.10
1	B	1482	PRO	C-N-CA	8.72	143.50	121.70
1	C	1837	ASN	CB-CA-C	7.36	125.12	110.40
1	B	1481	ARG	C-N-CA	6.49	149.24	122.00
1	B	2127	ARG	NE-CZ-NH1	-5.84	117.38	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1481	ARG	Peptide
1	A	1482	PRO	Peptide
1	A	1786	ASN	Mainchain
1	B	1481	ARG	Peptide
1	B	1482	PRO	Peptide
1	B	1786	ASN	Mainchain
1	C	1786	ASN	Mainchain

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	5491	0	5431	156	1
1	B	5421	0	5369	234	0
1	C	5387	0	5318	205	0
2	A	23	0	21	1	0
2	B	46	0	42	24	0
All	All	16368	0	16181	567	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (567) 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:1730:CYS:HA	1:A:1752:GLN:HE21	1.04	1.19
1:B:2004:ASP:OD2	1:B:2006:THR:HB	1.50	1.09
1:B:2148:ARG:CG	1:B:2148:ARG:HH11	1.70	1.05
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.54	1.05
1:B:2006:THR:HG23	1:C:1710:LEU:HA	1.42	1.01
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.25	0.99
1:C:1491:GLU:HG2	1:C:1491:GLU:O	1.63	0.96
1:B:1673:ASN:H	1:B:1673:ASN:HD22	1.04	0.95
1:C:2005:PRO:HD3	1:C:2014:MET:CE	1.96	0.95
1:C:2192:GLU:HA	1:C:2193:SER:HB3	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2080:ARG:O	1:A:2080:ARG:HG2	1.64	0.94
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.16	0.93
1:B:2000:TRP:CZ2	1:B:2014:MET:CE	2.51	0.93
1:B:2006:THR:CG2	1:C:1710:LEU:CA	2.46	0.93
1:A:1881:ARG:HG2	1:A:1881:ARG:HH11	1.32	0.93
1:B:1675:VAL:HG23	1:B:1677:THR:HG23	1.51	0.93
1:B:2006:THR:CG2	1:C:1710:LEU:HA	1.98	0.92
1:B:2145:GLU:OE2	1:B:2145:GLU:HA	1.70	0.91
1:C:2081:GLU:OE2	1:C:2081:GLU:HA	1.67	0.91
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.16	0.90
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.14	0.90
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	1.86	0.90
1:B:2006:THR:HG21	1:C:1710:LEU:N	1.85	0.89
1:B:2148:ARG:HH11	1:B:2148:ARG:HG3	1.38	0.88
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.20	0.87
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.56	0.87
1:C:1625:SER:HB3	1:C:1731:ARG:HH21	1.39	0.85
1:C:1580:ARG:HH11	1:C:1580:ARG:HG3	1.41	0.84
1:B:1852:THR:HG22	1:B:1854:SER:H	1.42	0.84
1:C:2005:PRO:HD3	1:C:2014:MET:HE3	1.60	0.84
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.26	0.82
1:C:1769:GLU:HG3	1:C:1769:GLU:O	1.79	0.82
1:B:2006:THR:CG2	1:C:1710:LEU:N	2.41	0.82
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.24	0.82
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.62	0.81
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.42	0.81
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	1.95	0.81
1:B:1730:CYS:O	1:B:1731:ARG:HB3	1.78	0.81
1:B:1562:ILE:HD11	1:B:1599:GLN:CB	2.11	0.81
1:B:1730:CYS:O	1:B:1730:CYS:SG	2.38	0.81
1:B:1480:LEU:O	1:B:1481:ARG:CG	2.30	0.80
1:B:2140:SER:O	1:B:2142:GLN:N	2.15	0.80
1:C:1674:SER:O	1:C:1694:ILE:HB	1.82	0.80
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.64	0.79
1:B:2148:ARG:HH11	1:B:2148:ARG:HG2	1.45	0.79
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.27	0.78
1:B:1602:GLU:OE1	1:B:1606:LYS:HD2	1.82	0.78
1:A:2080:ARG:O	1:A:2080:ARG:CG	2.30	0.77
1:C:1530:VAL:O	1:C:1530:VAL:HG23	1.85	0.77
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	1.66	0.76
1:B:2006:THR:HG21	1:C:1710:LEU:CA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2001:VAL:CG1	2:B:2240:GY3:H27B	2.15	0.76
1:B:2000:TRP:CZ2	1:B:2014:MET:HE2	2.19	0.76
1:B:1480:LEU:O	1:B:1481:ARG:CB	2.32	0.76
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.84	0.76
1:C:2097:HIS:O	1:C:2102:ARG:HG3	1.86	0.75
1:B:1675:VAL:HG23	1:B:1677:THR:CG2	2.15	0.75
1:C:2141:HIS:O	1:C:2142:GLN:HB2	1.85	0.75
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	1.69	0.75
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.31	0.75
1:C:2192:GLU:HA	1:C:2193:SER:CB	2.15	0.75
1:B:2189:LEU:HD13	1:B:2189:LEU:C	2.07	0.75
1:A:2189:LEU:O	1:A:2192:GLU:N	2.21	0.74
1:B:2001:VAL:HG21	2:B:2240:GY3:H21	1.69	0.73
1:C:1546:GLU:CD	1:C:1546:GLU:H	1.92	0.73
1:C:1540:ASN:HB2	1:C:1552:GLU:HG2	1.70	0.72
1:C:2192:GLU:CA	1:C:2193:SER:HB3	2.18	0.72
1:B:1673:ASN:HD22	1:B:1673:ASN:N	1.82	0.72
1:C:1546:GLU:N	1:C:1546:GLU:OE2	2.23	0.72
1:B:1562:ILE:HD11	1:B:1599:GLN:HB2	1.72	0.71
1:C:2192:GLU:CA	1:C:2193:SER:CB	2.67	0.71
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.89	0.71
1:A:1881:ARG:HG2	1:A:1881:ARG:NH1	1.99	0.71
1:C:1645:ASP:OD2	1:C:1648:ASN:HB2	1.90	0.70
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.38	0.70
1:B:2085:ILE:HG21	1:C:1650:ASP:HA	1.73	0.70
1:B:1657:TYR:CE2	1:B:1687:ARG:HG2	2.27	0.69
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.38	0.69
1:A:1987:ILE:HD12	1:A:2003:VAL:HG22	1.74	0.69
1:B:2083:LEU:N	1:B:2084:PRO:HD3	2.07	0.69
1:C:1852:THR:HG22	1:C:1854:SER:H	1.58	0.69
1:C:2141:HIS:O	1:C:2142:GLN:CB	2.42	0.68
1:A:1682:ILE:O	1:A:1683:ASN:C	2.32	0.68
1:C:2081:GLU:OE2	1:C:2081:GLU:CA	2.42	0.68
1:C:1654:GLN:HA	1:C:1654:GLN:OE1	1.93	0.68
1:C:2030:MET:CE	1:C:2034:LYS:HB2	2.24	0.68
1:B:2000:TRP:CZ2	1:B:2014:MET:HE3	2.29	0.67
1:B:1673:ASN:H	1:B:1673:ASN:ND2	1.85	0.67
1:A:1560:ASN:H	1:A:1560:ASN:ND2	1.88	0.67
1:A:1772:THR:H	1:A:1776:GLN:HE21	1.42	0.67
1:C:1580:ARG:HG3	1:C:1580:ARG:NH1	2.05	0.67
1:B:2014:MET:HG2	1:B:2109:ILE:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1480:LEU:O	1:B:1481:ARG:HB3	1.95	0.67
1:A:2136:ILE:HD11	1:A:2152:ILE:HG12	1.77	0.66
1:A:2014:MET:HG2	1:A:2109:ILE:HG22	1.76	0.66
1:B:2092:GLN:NE2	1:B:2092:GLN:HA	2.09	0.66
1:B:1852:THR:CG2	1:B:1854:SER:H	2.09	0.66
1:B:2148:ARG:HG3	1:B:2148:ARG:NH1	2.07	0.66
1:C:1814:ARG:O	1:C:1815:ASN:HB2	1.95	0.66
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.78	0.65
1:B:1648:ASN:O	1:B:1650:ASP:N	2.29	0.65
1:A:1881:ARG:NE	1:A:1943:GLU:OE2	2.26	0.65
1:B:1730:CYS:O	1:B:1731:ARG:CB	2.45	0.65
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.78	0.65
1:B:2000:TRP:CE2	1:B:2014:MET:HE3	2.32	0.65
1:C:1860:LEU:HD23	1:C:1948:MET:HE2	1.79	0.65
1:B:1786:ASN:HB3	1:B:1788:VAL:HG23	1.79	0.65
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.91	0.65
1:B:2089:ILE:HG22	1:B:2090:SER:N	2.11	0.65
1:A:1767:GLY:O	1:A:1768:ARG:HB2	1.98	0.64
1:A:1769:GLU:O	1:A:1769:GLU:CG	2.45	0.64
1:C:2040:LEU:HA	1:C:2043:THR:HG22	1.79	0.64
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.12	0.64
1:B:2006:THR:HG23	1:C:1710:LEU:CA	2.15	0.64
1:B:2036:ARG:O	1:B:2038:GLU:N	2.31	0.64
1:A:2192:GLU:OE1	1:A:2192:GLU:HA	1.98	0.63
1:B:1562:ILE:HD11	1:B:1599:GLN:CD	2.19	0.63
1:B:2000:TRP:CH2	1:B:2014:MET:CE	2.81	0.63
1:B:2001:VAL:HG11	2:B:2240:GY3:C27	2.28	0.63
1:B:2000:TRP:CH2	1:B:2014:MET:HE2	2.34	0.63
1:C:1909:ASN:ND2	1:C:1911:ASN:H	1.96	0.63
1:B:2189:LEU:HD13	1:B:2190:LYS:N	2.14	0.63
1:B:1668:LYS:HZ1	1:B:1669:PHE:HE2	1.45	0.63
1:B:2148:ARG:CG	1:B:2148:ARG:NH1	2.42	0.63
1:B:1675:VAL:CG2	1:B:1677:THR:CG2	2.76	0.63
1:B:1711:ILE:HD12	1:B:1739:LEU:HD11	1.81	0.63
1:C:1582:PHE:CD1	1:C:1619:ILE:HD13	2.33	0.63
1:A:2092:GLN:HA	1:A:2092:GLN:NE2	2.14	0.62
1:B:1657:TYR:CD2	1:B:1687:ARG:HG2	2.34	0.62
1:C:1909:ASN:HD22	1:C:1911:ASN:H	1.47	0.62
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	1.81	0.62
1:C:1675:VAL:HG23	1:C:1677:THR:CG2	2.29	0.62
1:C:1852:THR:CG2	1:C:1853:GLU:N	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:TRP:CD1	1:A:2000:TRP:C	2.73	0.62
1:C:1653:PHE:H	1:C:1653:PHE:HD2	1.47	0.62
1:B:2000:TRP:CE2	1:B:2014:MET:CE	2.82	0.62
1:C:2005:PRO:HD3	1:C:2014:MET:HE2	1.79	0.62
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.00	0.62
1:A:1954:ARG:HG3	1:A:1954:ARG:HH11	1.64	0.61
1:C:1499:LYS:HB3	1:C:1590:THR:HG22	1.80	0.61
1:B:1530:VAL:O	1:B:1530:VAL:HG13	2.00	0.61
1:B:2189:LEU:C	1:B:2189:LEU:CD1	2.69	0.61
1:C:1769:GLU:O	1:C:1769:GLU:CG	2.45	0.61
1:C:1675:VAL:HG23	1:C:1677:THR:HG22	1.82	0.61
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.36	0.61
1:A:1783:MET:O	1:A:1786:ASN:HB2	2.00	0.60
1:B:1536:PHE:HA	1:B:1572:LYS:HG3	1.83	0.60
1:C:1523:TRP:CE2	1:C:1574:PRO:HD3	2.36	0.60
1:B:1530:VAL:O	1:B:1530:VAL:CG1	2.49	0.60
1:A:1648:ASN:N	1:A:1649:PRO:CD	2.65	0.60
1:A:2133:GLU:OE1	1:A:2148:ARG:NH2	2.35	0.60
1:C:2015:TYR:HB3	1:C:2113:LEU:HD12	1.83	0.59
1:B:1819:PRO:HD2	1:B:1888:PRO:HG3	1.83	0.59
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.38	0.59
1:C:1623:ALA:HB2	1:C:1729:THR:CG2	2.31	0.59
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.00	0.59
1:B:1481:ARG:HB3	1:B:1492:TRP:CD1	2.38	0.59
1:A:1772:THR:H	1:A:1776:GLN:NE2	2.00	0.59
1:C:2192:GLU:N	1:C:2193:SER:HA	2.17	0.58
1:C:1644:ASN:OD1	1:C:1654:GLN:NE2	2.36	0.58
1:C:1860:LEU:CD2	1:C:1948:MET:CE	2.82	0.58
1:B:2081:GLU:O	1:B:2082:LEU:HB3	2.04	0.58
1:A:2048:ASP:OD1	1:A:2050:LYS:HB3	2.04	0.58
1:C:1540:ASN:CB	1:C:1552:GLU:HG2	2.34	0.58
1:C:1675:VAL:CG2	1:C:1677:THR:HG22	2.33	0.58
1:C:2005:PRO:CD	1:C:2014:MET:HE3	2.31	0.58
1:A:1560:ASN:HD22	1:A:1560:ASN:N	1.93	0.58
1:A:1905:ALA:HB1	1:A:1912:SER:O	2.04	0.58
1:C:1772:THR:H	1:C:1776:GLN:HE21	1.47	0.58
1:C:1860:LEU:CD2	1:C:1948:MET:HE1	2.33	0.58
1:C:1909:ASN:HD22	1:C:1909:ASN:C	2.06	0.58
1:B:2145:GLU:OE2	1:B:2145:GLU:CA	2.47	0.58
1:A:2081:GLU:OE2	1:A:2081:GLU:HA	2.04	0.57
1:C:2192:GLU:N	1:C:2193:SER:CA	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2162:SER:HB3	1:B:1797:LEU:HD13	1.85	0.57
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.69	0.57
1:C:1580:ARG:HH11	1:C:1580:ARG:CG	2.14	0.57
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.40	0.57
1:C:2154:ARG:HG3	1:C:2154:ARG:NH1	2.19	0.57
1:A:1677:THR:HA	1:A:1689:VAL:O	2.05	0.57
1:C:1745:ARG:NH1	1:C:1943:GLU:HG3	2.21	0.56
1:B:2084:PRO:O	1:B:2088:GLN:HG2	2.05	0.56
1:B:1792:THR:O	1:B:1802:LYS:HE3	2.05	0.56
2:B:3000:GY3:H26	1:C:1998:GLY:HA3	1.87	0.56
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.04	0.56
1:A:2093:PHE:O	1:A:2097:HIS:HD2	1.88	0.56
1:B:1996:ARG:O	1:B:1997:GLY:C	2.43	0.56
1:C:2041:LEU:CD2	1:C:2044:MET:HE1	2.36	0.56
1:C:2015:TYR:HB3	1:C:2113:LEU:CD1	2.36	0.56
1:B:2148:ARG:HG2	1:B:2148:ARG:NH1	2.18	0.56
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.89	0.55
1:C:1530:VAL:O	1:C:1530:VAL:CG2	2.53	0.55
1:A:1494:GLN:OE1	1:A:1496:LYS:HG3	2.07	0.55
1:A:1922:GLN:CD	1:A:1954:ARG:HH12	2.10	0.55
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.01	0.55
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.42	0.55
1:A:1540:ASN:CB	1:A:1552:GLU:HG2	2.37	0.54
1:B:1668:LYS:NZ	1:B:1669:PHE:HE2	2.05	0.54
1:B:2029:GLY:O	1:B:2033:ILE:HD12	2.08	0.54
1:B:2189:LEU:CD1	1:B:2190:LYS:N	2.70	0.54
1:A:2083:LEU:N	1:A:2084:PRO:HD2	2.23	0.54
1:C:2189:LEU:C	1:C:2191:LEU:H	2.10	0.54
1:B:1989:ILE:HG12	1:B:1995:LEU:HD22	1.88	0.54
1:A:1649:PRO:O	1:A:1651:LYS:N	2.40	0.54
1:A:1540:ASN:HB3	1:A:1552:GLU:HG2	1.90	0.54
1:C:1677:THR:HA	1:C:1689:VAL:O	2.08	0.54
1:C:2041:LEU:HA	1:C:2044:MET:CE	2.38	0.54
1:A:1651:LYS:HD2	1:A:1651:LYS:O	2.08	0.54
1:A:1875:LYS:HB2	1:A:1899:VAL:HG21	1.90	0.54
1:B:1509:TYR:CB	1:B:1557:PRO:HB3	2.37	0.54
1:A:1798:ALA:O	1:A:1802:LYS:HD3	2.08	0.53
1:A:1889:LEU:N	1:A:1889:LEU:HD23	2.23	0.53
1:B:2001:VAL:HG12	2:B:2240:GY3:H27B	1.90	0.53
1:A:1991:PRO:O	1:A:2019:ASN:O	2.26	0.53
1:C:2192:GLU:O	1:C:2192:GLU:CG	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:PRO:HG3	1:A:1846:MET:SD	2.49	0.53
1:B:1682:ILE:HG22	1:B:1682:ILE:O	2.07	0.53
1:A:1721:ASP:OD2	1:A:1814:ARG:NH1	2.41	0.53
1:C:2109:ILE:HD12	1:C:2111:LYS:O	2.09	0.53
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.74	0.53
1:B:2006:THR:HG21	1:C:1710:LEU:CB	2.39	0.53
1:C:1860:LEU:HD23	1:C:1948:MET:CE	2.38	0.53
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.09	0.53
1:B:1650:ASP:C	1:B:1652:GLY:N	2.62	0.53
1:B:1629:ILE:HG22	1:C:2024:VAL:HG11	1.91	0.53
1:A:1925:HIS:HB3	1:A:1926:PRO:HD2	1.90	0.52
1:B:1998:GLY:HA3	2:B:2240:GY3:H26	1.90	0.52
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.09	0.52
1:B:2083:LEU:H	1:B:2084:PRO:HD3	1.72	0.52
1:C:2040:LEU:O	1:C:2043:THR:HG22	2.10	0.52
1:C:2041:LEU:HA	1:C:2044:MET:HE2	1.91	0.52
1:B:1998:GLY:HA2	2:B:2240:GY3:C22	2.40	0.52
1:A:1741:ARG:HD2	1:A:1741:ARG:O	2.09	0.52
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.92	0.52
1:A:2085:ILE:O	1:A:2088:GLN:HB2	2.10	0.52
1:B:2000:TRP:CH2	1:B:2014:MET:HE3	2.45	0.52
1:B:1701:GLY:HA2	1:C:2024:VAL:HG23	1.92	0.51
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.42	0.51
1:B:1653:PHE:CD1	1:B:1653:PHE:O	2.64	0.51
1:B:1995:LEU:HG	1:B:2000:TRP:HA	1.91	0.51
1:B:2136:ILE:HD11	1:B:2152:ILE:HG23	1.91	0.51
1:A:1505:THR:HB	1:A:1730:CYS:HB2	1.92	0.51
1:B:1513:GLU:HA	1:B:1513:GLU:OE2	2.10	0.51
1:B:1894:VAL:HG22	1:B:1953:TRP:CE2	2.45	0.51
1:C:1813:LYS:HG2	1:C:1816:MET:HG3	1.92	0.51
1:B:2006:THR:HG21	1:C:1710:LEU:HB2	1.93	0.51
1:A:1922:GLN:CD	1:A:1954:ARG:NH1	2.64	0.51
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.58	0.51
1:B:2040:LEU:HD11	1:B:2086:TYR:HB3	1.93	0.51
1:A:1670:ASP:O	1:A:1671:LYS:HG3	2.10	0.51
1:C:1663:MET:HE3	1:C:1688:PHE:HB3	1.93	0.51
1:A:1619:ILE:N	1:A:1619:ILE:CD1	2.74	0.50
1:B:1679:ARG:HG2	1:B:1679:ARG:HH11	1.76	0.50
1:B:1509:TYR:CG	1:B:1557:PRO:HB3	2.47	0.50
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.92	0.50
1:C:1852:THR:HB	1:C:1855:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1669:PHE:N	1:B:1669:PHE:CD2	2.76	0.50
1:B:2141:HIS:O	1:B:2190:LYS:HE3	2.10	0.50
1:C:2036:ARG:HH21	1:C:2037:ARG:HD2	1.76	0.50
1:A:1619:ILE:N	1:A:1619:ILE:HD13	2.27	0.50
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.44	0.50
1:B:2189:LEU:C	1:B:2191:LEU:H	2.15	0.50
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.10	0.50
1:A:1624:ASN:HD22	1:A:1626:GLY:H	1.59	0.50
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.11	0.50
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	1.93	0.50
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.42	0.50
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.42	0.50
1:C:2040:LEU:CA	1:C:2043:THR:HG22	2.41	0.49
1:A:2180:LYS:HG3	1:B:1482:PRO:HD3	1.93	0.49
1:B:1697:GLU:HG3	1:B:1698:ASP:N	2.27	0.49
1:B:1925:HIS:O	1:B:1926:PRO:C	2.51	0.49
1:C:1701:GLY:O	1:C:1704:CYS:HB2	2.12	0.49
1:B:2001:VAL:CG1	2:B:2240:GY3:C27	2.85	0.49
1:B:1636:VAL:HB	1:B:1637:PRO:CD	2.41	0.49
1:C:1491:GLU:O	1:C:1492:TRP:O	2.30	0.49
1:B:1769:GLU:CG	1:B:1769:GLU:O	2.60	0.49
1:B:1968:LEU:CD1	1:C:1756:LEU:HD21	2.43	0.49
1:A:1769:GLU:O	1:A:1769:GLU:HG3	2.12	0.49
1:B:1902:LEU:HD12	1:B:1903:ILE:N	2.26	0.49
1:C:1852:THR:CG2	1:C:1853:GLU:H	2.24	0.49
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.61	0.49
1:A:1881:ARG:NH1	1:A:1881:ARG:CG	2.72	0.49
1:B:1494:GLN:NE2	1:B:1496:LYS:H	2.01	0.49
1:B:1644:ASN:HD21	1:B:1654:GLN:HB2	1.77	0.49
1:C:1582:PHE:HD1	1:C:1619:ILE:HD13	1.76	0.49
1:A:2142:GLN:NE2	1:A:2190:LYS:HG2	2.27	0.49
1:B:1810:VAL:HG13	1:B:1811:PRO:HD2	1.95	0.49
1:B:1852:THR:HG22	1:B:1855:GLY:H	1.78	0.49
1:C:2191:LEU:C	1:C:2193:SER:HB2	2.32	0.49
1:B:1545:ASP:HB2	1:B:1546:GLU:OE1	2.13	0.49
1:B:2006:THR:CG2	1:C:1710:LEU:HB2	2.43	0.49
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.60	0.49
1:C:2041:LEU:HD23	1:C:2044:MET:HE1	1.95	0.49
1:A:1922:GLN:OE1	1:A:1954:ARG:NH1	2.46	0.48
1:B:2147:SER:O	1:B:2148:ARG:C	2.51	0.48
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2190:LYS:O	1:C:2190:LYS:HG2	2.12	0.48
1:A:1646:ALA:O	1:A:1647:ALA:HB3	2.13	0.48
1:A:2194:PHE:CD2	1:A:2195:ALA:N	2.81	0.48
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.48	0.48
1:C:1644:ASN:ND2	1:C:1651:LYS:O	2.46	0.48
1:B:1797:LEU:HD22	1:B:1801:GLU:HG3	1.94	0.48
1:B:1925:HIS:HB3	1:B:1926:PRO:HD2	1.95	0.48
1:B:2006:THR:CG2	1:C:1710:LEU:CB	2.92	0.48
1:C:1674:SER:O	1:C:1694:ILE:CB	2.57	0.48
1:A:1482:PRO:HG2	1:A:1489:VAL:HG21	1.96	0.48
1:A:1589:ILE:O	1:A:1589:ILE:HD12	2.13	0.48
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.77	0.48
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	1.96	0.48
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.94	0.48
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.11	0.48
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	1.96	0.48
1:B:1629:ILE:CG2	1:C:2024:VAL:HG11	2.44	0.48
1:B:2089:ILE:CG2	1:B:2090:SER:N	2.77	0.48
1:A:2137:LYS:O	1:A:2138:ARG:C	2.50	0.48
1:A:2155:ILE:O	1:A:2158:TRP:HB2	2.14	0.48
1:B:1480:LEU:O	1:B:1481:ARG:HG2	2.13	0.48
1:C:2159:TYR:N	1:C:2159:TYR:CD2	2.81	0.48
1:A:1889:LEU:HD23	1:A:1889:LEU:H	1.79	0.47
1:A:2048:ASP:OD1	1:A:2050:LYS:CB	2.62	0.47
1:C:2191:LEU:HD13	1:C:2191:LEU:O	2.14	0.47
1:C:2145:GLU:OE1	1:C:2145:GLU:HA	2.14	0.47
1:A:1909:ASN:C	1:A:1909:ASN:OD1	2.52	0.47
1:B:2085:ILE:N	1:B:2085:ILE:HD13	2.28	0.47
1:C:1667:LYS:HB3	1:C:1667:LYS:HE2	1.63	0.47
1:B:1739:LEU:HA	1:B:1739:LEU:HD23	1.65	0.47
1:B:1996:ARG:HA	1:B:2023:GLY:O	2.14	0.47
1:C:1829:ARG:HB2	1:C:1830:PRO:HD2	1.97	0.47
1:A:1587:ASN:ND2	1:A:1624:ASN:HB3	2.29	0.47
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.46	0.47
1:B:1638:LEU:C	1:B:1638:LEU:HD12	2.34	0.47
1:C:2032:GLY:O	1:C:2036:ARG:HD2	2.14	0.47
1:A:1909:ASN:O	1:A:1910:PRO:C	2.52	0.47
1:B:1537:PHE:CD1	1:B:1537:PHE:C	2.88	0.47
1:B:1624:ASN:HD22	1:B:1626:GLY:N	2.05	0.47
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.62	0.47
1:B:1562:ILE:HD11	1:B:1599:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1634:GLU:HG2	1:B:1635:ILE:HG12	1.95	0.47
1:B:1650:ASP:O	1:B:1652:GLY:N	2.48	0.47
1:C:1491:GLU:O	1:C:1491:GLU:CG	2.44	0.47
1:B:1954:ARG:NH1	1:B:1994:GLU:OE1	2.48	0.47
1:C:1639:PHE:CD1	1:C:1639:PHE:C	2.88	0.47
1:C:1659:THR:O	1:C:1662:GLY:N	2.36	0.47
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.14	0.47
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.78	0.47
1:B:2114:GLU:O	1:B:2115:TRP:C	2.53	0.47
1:B:2138:ARG:HB3	1:B:2186:LEU:HD13	1.97	0.47
1:C:1653:PHE:N	1:C:1653:PHE:CD2	2.82	0.47
1:A:1925:HIS:O	1:A:1926:PRO:C	2.53	0.47
1:C:1622:ALA:O	1:C:1729:THR:HG22	2.14	0.47
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.15	0.46
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.50	0.46
1:B:1998:GLY:CA	2:B:2240:GY3:C24	2.93	0.46
1:A:1770:VAL:HG22	1:A:1771:TYR:CD1	2.50	0.46
1:B:1900:GLU:HB3	1:B:1916:LEU:HD11	1.97	0.46
1:A:2189:LEU:O	1:A:2191:LEU:N	2.49	0.46
1:C:2040:LEU:HA	1:C:2043:THR:CG2	2.43	0.46
1:C:2050:LYS:HE2	1:C:2050:LYS:HB2	1.62	0.46
1:B:1824:LYS:HE2	1:B:1824:LYS:HB3	1.44	0.46
1:A:2142:GLN:O	1:A:2143:VAL:HG23	2.16	0.46
2:A:3000:GY3:H28A	2:A:3000:GY3:O12	2.16	0.46
1:B:1963:MET:HE1	1:C:1783:MET:CE	2.46	0.46
1:B:2044:MET:O	1:B:2047:LEU:C	2.54	0.46
1:C:1759:ALA:N	1:C:1760:PRO:CD	2.78	0.46
1:C:2164:ASP:C	1:C:2164:ASP:OD1	2.54	0.46
1:A:1573:THR:HB	1:A:1574:PRO:HD2	1.96	0.46
1:B:1727:LEU:HG	1:B:1729:THR:HG23	1.97	0.46
1:B:2143:VAL:O	1:B:2145:GLU:N	2.49	0.46
2:B:2240:GY3:C7	1:C:1734:GLY:HA3	2.46	0.46
1:B:1644:ASN:ND2	1:B:1654:GLN:HB2	2.31	0.45
1:B:1763:ASN:ND2	1:B:1770:VAL:H	2.13	0.45
1:C:1591:PHE:C	1:C:1591:PHE:CD2	2.89	0.45
1:A:1480:LEU:HG	1:A:1481:ARG:HD3	1.98	0.45
1:A:2142:GLN:HB3	1:A:2143:VAL:H	1.55	0.45
1:B:1659:THR:O	1:B:1660:SER:C	2.55	0.45
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.15	0.45
1:C:1659:THR:O	1:C:1660:SER:C	2.55	0.45
1:A:1480:LEU:HB3	1:A:1481:ARG:H	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1562:ILE:CD1	1:B:1599:GLN:HB2	2.45	0.45
1:B:1906:ASP:HA	1:B:1907:PRO:HD3	1.86	0.45
1:C:1894:VAL:HG22	1:C:1953:TRP:CZ2	2.51	0.45
1:B:1511:PHE:O	1:B:1512:PRO:C	2.53	0.45
1:B:1734:GLY:HA3	2:B:3000:GY3:C7	2.46	0.45
1:C:1860:LEU:HD21	1:C:1948:MET:HE1	1.98	0.45
1:A:1846:MET:HE3	1:A:2115:TRP:CH2	2.52	0.45
1:A:2152:ILE:HD13	1:A:2152:ILE:HA	1.58	0.45
1:A:2008:ASN:C	1:A:2008:ASN:HD22	2.20	0.45
1:B:1562:ILE:HD11	1:B:1599:GLN:HB3	1.95	0.45
1:B:1572:LYS:HB3	1:B:1577:PRO:O	2.17	0.45
1:B:1998:GLY:HA3	2:B:2240:GY3:C24	2.47	0.45
1:A:1767:GLY:O	1:A:1768:ARG:CB	2.64	0.45
1:A:1786:ASN:HB3	1:A:1788:VAL:H	1.81	0.45
1:A:2033:ILE:HG22	1:A:2034:LYS:HD3	1.99	0.45
1:C:1681:VAL:O	1:C:1681:VAL:HG23	2.17	0.45
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.99	0.45
1:B:2092:GLN:HA	1:B:2092:GLN:HE21	1.82	0.45
2:B:2240:GY3:H9	1:C:1626:GLY:HA3	1.99	0.45
1:C:1703:GLU:HG2	1:C:1704:CYS:N	2.32	0.45
1:A:1648:ASN:N	1:A:1649:PRO:HD3	2.33	0.44
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.17	0.44
1:C:2000:TRP:CD1	1:C:2000:TRP:C	2.91	0.44
1:A:1648:ASN:H	1:A:1649:PRO:HD3	1.81	0.44
1:A:1775:LEU:HD12	1:A:1775:LEU:HA	1.77	0.44
1:C:2190:LYS:O	1:C:2190:LYS:CG	2.65	0.44
1:A:1645:ASP:OD2	1:A:1645:ASP:C	2.56	0.44
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.62	0.44
1:A:1832:ASP:HB2	1:A:1858:TYR:N	2.32	0.44
1:A:1866:PHE:CE1	1:A:1868:GLU:HB2	2.52	0.44
1:A:2178:ASN:O	1:A:2179:TYR:C	2.55	0.44
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.52	0.44
1:B:2001:VAL:HG22	1:C:1708:SER:HB2	1.98	0.44
1:C:1741:ARG:O	1:C:1744:GLN:N	2.38	0.44
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.63	0.44
1:C:2160:PRO:C	1:C:2162:SER:H	2.20	0.44
1:B:1997:GLY:HA2	2:B:2240:GY3:H29A	1.99	0.44
1:B:2004:ASP:HA	1:B:2005:PRO:HD3	1.88	0.44
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.55	0.44
1:A:1592:LYS:C	1:A:1593:ILE:HG12	2.37	0.44
1:B:1524:LYS:HD2	1:B:1524:LYS:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1833:PHE:O	1:B:1833:PHE:CD2	2.71	0.44
1:A:1843:VAL:O	1:A:1847:ILE:HG13	2.18	0.44
1:B:1998:GLY:HA2	2:B:2240:GY3:C21	2.47	0.44
1:A:2093:PHE:O	1:A:2097:HIS:CD2	2.68	0.44
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.33	0.44
1:B:1480:LEU:O	1:B:1481:ARG:HG3	2.17	0.44
1:B:2011:GLN:HE22	1:B:2148:ARG:HH22	1.65	0.44
1:B:2112:GLU:O	1:B:2113:LEU:HD23	2.17	0.44
1:A:1664:GLU:O	1:A:1665:THR:C	2.55	0.43
1:A:1730:CYS:O	1:A:1731:ARG:HB3	2.17	0.43
1:A:1749:VAL:O	1:A:1750:GLU:C	2.57	0.43
1:B:1576:TYR:CZ	1:B:1812:ALA:HB2	2.53	0.43
1:B:1894:VAL:CG2	1:B:1953:TRP:CE2	3.01	0.43
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.99	0.43
1:C:1527:SER:C	1:C:1529:ASP:H	2.21	0.43
1:A:1657:TYR:CD2	1:A:1687:ARG:HD2	2.52	0.43
1:A:2048:ASP:HB3	1:A:2051:TYR:H	1.84	0.43
1:B:1786:ASN:OD1	1:C:1964:PHE:O	2.37	0.43
1:B:2131:ASN:HB3	1:B:2175:ILE:HG21	2.00	0.43
1:C:1527:SER:C	1:C:1529:ASP:N	2.71	0.43
1:C:1909:ASN:HD22	1:C:1910:PRO:N	2.16	0.43
1:A:1633:GLU:OE1	1:A:1633:GLU:HA	2.18	0.43
1:B:1837:ASN:H	1:B:1837:ASN:ND2	2.17	0.43
1:C:1644:ASN:HD21	1:C:1652:GLY:HA3	1.82	0.43
1:A:1776:GLN:O	1:A:1782:ILE:CD1	2.66	0.43
1:B:1636:VAL:HB	1:B:1637:PRO:HD3	2.01	0.43
1:B:1745:ARG:HD3	1:B:1943:GLU:OE2	2.19	0.43
1:B:2132:GLU:OE2	1:B:2159:TYR:OH	2.30	0.43
1:C:2121:PHE:CD2	1:C:2121:PHE:C	2.91	0.43
1:A:1494:GLN:NE2	1:A:1558:GLY:HA3	2.34	0.43
1:B:1759:ALA:O	1:B:1760:PRO:C	2.57	0.43
2:B:2240:GY3:O12	1:C:1734:GLY:HA3	2.19	0.43
1:A:1889:LEU:N	1:A:1889:LEU:CD2	2.82	0.43
1:B:1682:ILE:HD13	1:B:1682:ILE:HA	1.69	0.43
1:B:1546:GLU:HG2	1:B:1547:ASN:H	1.83	0.43
1:B:1998:GLY:CA	2:B:2240:GY3:C23	2.96	0.43
1:C:1925:HIS:H	1:C:1928:SER:HB3	1.84	0.43
1:C:2041:LEU:HD23	1:C:2044:MET:CE	2.49	0.43
1:C:2085:ILE:HD12	1:C:2085:ILE:HA	1.92	0.43
1:A:1954:ARG:HH11	1:A:1954:ARG:CG	2.28	0.43
1:A:2156:ARG:HB3	1:A:2165:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1902:LEU:HD12	1:B:1903:ILE:H	1.83	0.43
1:C:1550:LEU:HD12	1:C:1550:LEU:HA	1.78	0.43
1:C:1995:LEU:HG	1:C:2000:TRP:HA	2.00	0.43
1:C:2040:LEU:C	1:C:2043:THR:HG22	2.39	0.43
1:C:2192:GLU:N	1:C:2193:SER:CB	2.81	0.43
1:C:2152:ILE:O	1:C:2156:ARG:HG3	2.19	0.43
1:A:1664:GLU:O	1:A:1666:LEU:N	2.52	0.42
1:B:1963:MET:CE	1:C:1783:MET:CE	2.97	0.42
1:C:1747:ILE:HD12	1:C:1803:ILE:HG13	2.01	0.42
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.84	0.42
1:C:1772:THR:N	1:C:1776:GLN:HE22	2.02	0.42
1:B:1947:MET:HE3	1:B:1985:ILE:HG23	2.01	0.42
1:C:1623:ALA:HB2	1:C:1729:THR:HG22	1.98	0.42
1:C:1667:LYS:HG2	1:C:1672:GLU:OE1	2.19	0.42
1:C:2152:ILE:H	1:C:2152:ILE:HG12	1.68	0.42
1:A:1649:PRO:O	1:A:1650:ASP:C	2.57	0.42
1:A:2040:LEU:O	1:A:2041:LEU:C	2.57	0.42
1:A:2134:TYR:HD2	1:A:2135:LEU:HD13	1.84	0.42
1:B:2082:LEU:C	1:B:2084:PRO:HD2	2.39	0.42
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.49	0.42
1:C:1526:PHE:CE2	1:C:1821:LEU:HD11	2.54	0.42
1:C:2154:ARG:HH11	1:C:2154:ARG:CG	2.33	0.42
1:A:1749:VAL:O	1:A:1752:GLN:HG2	2.20	0.42
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.23	0.42
1:C:1990:PRO:HB2	1:C:1991:PRO:HD2	2.02	0.42
1:A:1874:ALA:HB3	1:A:1931:LYS:HD3	2.00	0.42
1:B:1947:MET:HE2	1:B:1985:ILE:HG12	2.02	0.42
1:C:2149:LEU:H	1:C:2149:LEU:HG	1.43	0.42
1:A:1659:THR:O	1:A:1660:SER:C	2.57	0.42
1:C:1955:GLY:HA2	1:C:1999:SER:OG	2.20	0.42
1:B:1672:GLU:H	1:B:1672:GLU:HG3	1.52	0.42
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.01	0.42
1:A:1569:ILE:O	1:A:1581:GLN:HA	2.20	0.42
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.19	0.42
1:C:1672:GLU:C	1:C:1674:SER:H	2.23	0.42
1:C:1842:ASP:OD1	1:C:1844:ARG:HD2	2.20	0.42
1:C:2036:ARG:HE	1:C:2036:ARG:HB3	1.68	0.42
1:C:2041:LEU:CD2	1:C:2044:MET:CE	2.97	0.42
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.35	0.42
1:A:1817:PRO:HB3	1:B:1486:PRO:HA	2.01	0.42
1:A:1883:ARG:HG3	1:A:1883:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2106:LYS:NZ	1:C:1698:ASP:OD1	2.42	0.42
1:A:1787:GLY:HA3	1:A:1873:TRP:CE3	2.55	0.41
1:B:1734:GLY:HA3	2:B:3000:GY3:O12	2.20	0.41
1:B:1963:MET:O	1:B:1964:PHE:C	2.58	0.41
1:B:1998:GLY:HA2	2:B:2240:GY3:C23	2.50	0.41
1:C:2046:ARG:HG3	1:C:2047:LEU:HD13	2.02	0.41
1:B:1650:ASP:C	1:B:1652:GLY:H	2.22	0.41
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.20	0.41
1:B:2152:ILE:H	1:B:2152:ILE:HG13	1.69	0.41
1:C:1669:PHE:O	1:C:1671:LYS:HG3	2.21	0.41
1:A:1499:LYS:HD3	1:A:1499:LYS:HA	1.80	0.41
1:A:1587:ASN:ND2	1:A:1620:TYR:OH	2.48	0.41
1:C:1674:SER:O	1:C:1694:ILE:HG13	2.20	0.41
1:C:1731:ARG:HB2	1:C:1753:PRO:HG2	2.01	0.41
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	2.02	0.41
1:A:1530:VAL:O	1:A:1530:VAL:HG13	2.21	0.41
1:A:1903:ILE:HA	1:A:1904:PRO:HD3	1.95	0.41
1:A:2139:LEU:HD23	1:A:2139:LEU:HA	1.77	0.41
1:B:1877:VAL:HG13	1:B:1931:LYS:HD3	2.02	0.41
1:B:2025:LEU:HD21	2:B:2240:GY3:H2A	2.02	0.41
1:C:1496:LYS:O	1:C:1590:THR:HG21	2.21	0.41
1:A:1756:LEU:HD23	1:A:1756:LEU:HA	1.65	0.41
1:B:1639:PHE:HA	1:B:1658:LEU:HD12	2.02	0.41
1:C:2106:LYS:HD2	1:C:2106:LYS:HA	1.72	0.41
1:C:2139:LEU:HD21	1:C:2154:ARG:HD2	2.01	0.41
1:B:2024:VAL:HG12	2:B:2240:GY3:H2	2.02	0.41
1:B:2081:GLU:O	1:B:2081:GLU:HG3	2.20	0.41
1:C:1651:LYS:O	1:C:1652:GLY:O	2.38	0.41
1:A:1995:LEU:HG	1:A:2000:TRP:HA	2.03	0.41
1:A:2084:PRO:O	1:A:2088:GLN:HG2	2.21	0.41
1:B:1480:LEU:HB3	1:B:1481:ARG:H	1.74	0.41
1:B:1526:PHE:CE2	1:B:1821:LEU:HD11	2.54	0.41
1:B:1734:GLY:HA2	2:B:3000:GY3:H25	2.01	0.41
1:B:2001:VAL:HG21	2:B:2240:GY3:C21	2.45	0.41
1:B:2096:LEU:HD23	1:B:2099:ARG:CZ	2.51	0.41
1:C:2160:PRO:O	1:C:2162:SER:N	2.54	0.41
1:B:1668:LYS:HB3	1:B:1668:LYS:HE2	1.35	0.41
1:A:1925:HIS:HB3	1:A:1926:PRO:CD	2.51	0.40
1:A:2158:TRP:CD1	1:A:2185:LYS:HE3	2.56	0.40
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.20	0.40
1:C:1639:PHE:HA	1:C:1658:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2104:VAL:O	1:C:2105:ALA:C	2.60	0.40
1:C:2192:GLU:O	1:C:2192:GLU:HG2	2.21	0.40
1:A:1726:THR:HG21	1:A:1740:VAL:HG22	2.02	0.40
1:B:1602:GLU:OE1	1:B:1606:LYS:CD	2.62	0.40
1:C:1673:ASN:OD1	1:C:1673:ASN:O	2.40	0.40
1:A:1664:GLU:C	1:A:1666:LEU:N	2.73	0.40
1:A:1875:LYS:HB2	1:A:1899:VAL:CG2	2.51	0.40
1:B:1968:LEU:HD12	1:B:1968:LEU:HA	1.79	0.40
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.20	0.40
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.57	0.40
1:A:1664:GLU:O	1:A:1667:LYS:N	2.54	0.40
1:B:1781:GLN:NE2	1:B:1781:GLN:H	2.19	0.40
1:B:2110:SER:O	1:B:2111:LYS:HG2	2.21	0.40
1:C:1527:SER:O	1:C:1529:ASP:N	2.54	0.40
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.38	0.40
1:A:1741:ARG:CZ	1:A:1744:GLN:HE22	2.35	0.40
1:A:2080:ARG:O	1:A:2080:ARG:NE	2.54	0.40
1:A:2082:LEU:C	1:A:2084:PRO:HD2	2.41	0.40
1:B:1629:ILE:HG22	1:C:2024:VAL:CG1	2.51	0.40
1:B:1729:THR:O	1:B:1730:CYS:CB	2.69	0.40
1:B:1998:GLY:HA3	2:B:2240:GY3:C23	2.52	0.40
1:B:2180:LYS:C	1:B:2182:LEU:N	2.75	0.40
1:C:1511:PHE:O	1:C:1514:LEU:N	2.55	0.40
1:C:1837:ASN:OD1	1:C:1992:THR:HG22	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1717:ARG:NH2	1:A:2007:ILE:O[2_555]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	684/764 (90%)	621 (91%)	48 (7%)	15 (2%)	6	22
1	B	676/764 (88%)	601 (89%)	55 (8%)	20 (3%)	4	15
1	C	671/764 (88%)	615 (92%)	46 (7%)	10 (2%)	10	33
All	All	2031/2292 (89%)	1837 (90%)	149 (7%)	45 (2%)	6	22

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	ASP
1	A	2190	LYS
1	B	1481	ARG
1	B	1651	LYS
1	B	1730	CYS
1	B	2037	ARG
1	B	2141	HIS
1	B	2143	VAL
1	C	1492	TRP
1	C	1683	ASN
1	C	2142	GLN
1	C	2190	LYS
1	A	1683	ASN
1	A	1768	ARG
1	A	2049	ASP
1	B	1838	ASP
1	B	2082	LEU
1	B	2144	GLY
1	B	2148	ARG
1	C	1652	GLY
1	C	1660	SER
1	C	2161	ALA
1	A	1670	ASP
1	A	1912	SER
1	A	2142	GLN
1	A	2144	GLY
1	A	2187	LYS
1	B	1649	PRO
1	B	1670	ASP
1	B	1731	ARG
1	B	2115	TRP
1	B	2180	LYS

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Mol	Chain	Res	Type
1	A	1671	LYS
1	A	1910	PRO
1	B	1660	SER
1	B	1744	GLN
1	B	2190	LYS
1	C	1528	ALA
1	C	1744	GLN
1	A	1660	SER
1	A	2152	ILE
1	B	1671	LYS
1	B	1997	GLY
1	A	1649	PRO
1	C	1684	GLY

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	584/654 (89%)	484 (83%)	100 (17%)	2	6
1	B	577/654 (88%)	490 (85%)	87 (15%)	3	9
1	C	573/654 (88%)	488 (85%)	85 (15%)	3	9
All	All	1734/1962 (88%)	1462 (84%)	272 (16%)	2	8

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1481	ARG
1	A	1483	ILE
1	A	1490	LYS
1	A	1499	LYS
1	A	1522	GLN
1	A	1536	PHE
1	A	1539	SER
1	A	1549	GLU
1	A	1552	GLU

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Mol	Chain	Res	Type
1	A	1554	GLU
1	A	1556	GLU
1	A	1560	ASN
1	A	1568	LYS
1	A	1578	ARG
1	A	1585	VAL
1	A	1589	ILE
1	A	1593	ILE
1	A	1602	GLU
1	A	1616	ILE
1	A	1618	ARG
1	A	1619	ILE
1	A	1629	ILE
1	A	1640	GLN
1	A	1645	ASP
1	A	1648	ASN
1	A	1650	ASP
1	A	1651	LYS
1	A	1659	THR
1	A	1660	SER
1	A	1666	LEU
1	A	1668	LYS
1	A	1673	ASN
1	A	1679	ARG
1	A	1685	GLU
1	A	1687	ARG
1	A	1730	CYS
1	A	1732	SER
1	A	1757	THR
1	A	1769	GLU
1	A	1775	LEU
1	A	1781	GLN
1	A	1794	VAL
1	A	1802	LYS
1	A	1820	ILE
1	A	1822	GLU
1	A	1826	THR
1	A	1839	GLU
1	A	1840	THR
1	A	1871	SER
1	A	1877	VAL
1	A	1878	VAL

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Mol	Chain	Res	Type
1	A	1879	VAL
1	A	1881	ARG
1	A	1884	LEU
1	A	1897	ARG
1	A	1906	ASP
1	A	1915	THR
1	A	1918	GLN
1	A	1924	TRP
1	A	1930	PHE
1	A	1950	LEU
1	A	1980	ASP
1	A	1995	LEU
1	A	1996	ARG
1	A	1999	SER
1	A	2002	VAL
1	A	2003	VAL
1	A	2008	ASN
1	A	2014	MET
1	A	2026	GLU
1	A	2028	GLN
1	A	2035	PHE
1	A	2037	ARG
1	A	2041	LEU
1	A	2044	MET
1	A	2046	ARG
1	A	2048	ASP
1	A	2049	ASP
1	A	2080	ARG
1	A	2081	GLU
1	A	2083	LEU
1	A	2089	ILE
1	A	2091	LEU
1	A	2128	ARG
1	A	2135	LEU
1	A	2137	LYS
1	A	2139	LEU
1	A	2141	HIS
1	A	2142	GLN
1	A	2145	GLU
1	A	2148	ARG
1	A	2149	LEU
1	A	2152	ILE

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Mol	Chain	Res	Type
1	A	2154	ARG
1	A	2185	LYS
1	A	2187	LYS
1	A	2189	LEU
1	A	2190	LYS
1	A	2191	LEU
1	A	2194	PHE
1	B	1480	LEU
1	B	1481	ARG
1	B	1516	ARG
1	B	1529	ASP
1	B	1530	VAL
1	B	1531	LYS
1	B	1534	ASP
1	B	1536	PHE
1	B	1562	ILE
1	B	1568	LYS
1	B	1571	VAL
1	B	1572	LYS
1	B	1583	VAL
1	B	1589	ILE
1	B	1602	GLU
1	B	1606	LYS
1	B	1616	ILE
1	B	1629	ILE
1	B	1644	ASN
1	B	1648	ASN
1	B	1651	LYS
1	B	1653	PHE
1	B	1658	LEU
1	B	1668	LYS
1	B	1669	PHE
1	B	1672	GLU
1	B	1673	ASN
1	B	1679	ARG
1	B	1680	THR
1	B	1682	ILE
1	B	1685	GLU
1	B	1689	VAL
1	B	1691	LYS
1	B	1697	GLU
1	B	1726	THR

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Mol	Chain	Res	Type
1	B	1731	ARG
1	B	1757	THR
1	B	1769	GLU
1	B	1781	GLN
1	B	1792	THR
1	B	1797	LEU
1	B	1822	GLU
1	B	1824	LYS
1	B	1836	THR
1	B	1837	ASN
1	B	1843	VAL
1	B	1852	THR
1	B	1854	SER
1	B	1871	SER
1	B	1900	GLU
1	B	1911	ASN
1	B	1915	THR
1	B	1924	TRP
1	B	1930	PHE
1	B	1968	LEU
1	B	1980	ASP
1	B	1995	LEU
1	B	2003	VAL
1	B	2006	THR
1	B	2011	GLN
1	B	2021	ARG
1	B	2034	LYS
1	B	2035	PHE
1	B	2037	ARG
1	B	2039	LYS
1	B	2043	THR
1	B	2046	ARG
1	B	2082	LEU
1	B	2085	ILE
1	B	2089	ILE
1	B	2092	GLN
1	B	2101	SER
1	B	2127	ARG
1	B	2128	ARG
1	B	2133	GLU
1	B	2137	LYS
1	B	2143	VAL

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Mol	Chain	Res	Type
1	B	2145	GLU
1	B	2147	SER
1	B	2148	ARG
1	B	2149	LEU
1	B	2152	ILE
1	B	2165	HIS
1	B	2166	GLU
1	B	2180	LYS
1	B	2185	LYS
1	B	2189	LEU
1	C	1499	LYS
1	C	1508	VAL
1	C	1516	ARG
1	C	1520	SER
1	C	1522	GLN
1	C	1534	ASP
1	C	1536	PHE
1	C	1546	GLU
1	C	1550	LEU
1	C	1552	GLU
1	C	1560	ASN
1	C	1565	VAL
1	C	1568	LYS
1	C	1571	VAL
1	C	1580	ARG
1	C	1585	VAL
1	C	1613	LYS
1	C	1616	ILE
1	C	1618	ARG
1	C	1629	ILE
1	C	1634	GLU
1	C	1643	TRP
1	C	1644	ASN
1	C	1648	ASN
1	C	1653	PHE
1	C	1654	GLN
1	C	1664	GLU
1	C	1667	LYS
1	C	1677	THR
1	C	1680	THR
1	C	1685	GLU
1	C	1686	GLU

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Mol	Chain	Res	Type
1	C	1687	ARG
1	C	1690	ILE
1	C	1731	ARG
1	C	1741	ARG
1	C	1764	LYS
1	C	1765	MET
1	C	1768	ARG
1	C	1769	GLU
1	C	1770	VAL
1	C	1773	SER
1	C	1777	LEU
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1802	LYS
1	C	1824	LYS
1	C	1838	ASP
1	C	1843	VAL
1	C	1877	VAL
1	C	1879	VAL
1	C	1900	GLU
1	C	1909	ASN
1	C	1911	ASN
1	C	1914	GLU
1	C	1916	LEU
1	C	1924	TRP
1	C	1930	PHE
1	C	1961	ARG
1	C	1968	LEU
1	C	1980	ASP
1	C	2028	GLN
1	C	2031	VAL
1	C	2036	ARG
1	C	2037	ARG
1	C	2038	GLU
1	C	2046	ARG
1	C	2047	LEU
1	C	2050	LYS
1	C	2081	GLU
1	C	2083	LEU
1	C	2088	GLN
1	C	2101	SER

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Mol	Chain	Res	Type
1	C	2102	ARG
1	C	2106	LYS
1	C	2111	LYS
1	C	2128	ARG
1	C	2149	LEU
1	C	2152	ILE
1	C	2180	LYS
1	C	2185	LYS
1	C	2191	LEU
1	C	2192	GLU
1	C	2193	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1673	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1918	GLN
1	A	1965	ASN
1	A	2008	ASN
1	A	2092	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	GLN
1	A	2165	HIS
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1581	GLN
1	B	1587	ASN
1	B	1599	GLN

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Mol	Chain	Res	Type
1	B	1605	ASN
1	B	1624	ASN
1	B	1673	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1781	GLN
1	B	1815	ASN
1	B	1837	ASN
1	B	1925	HIS
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2092	GLN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1648	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1786	ASN
1	C	1815	ASN
1	C	1909	ASN
1	C	1918	GLN
1	C	1922	GLN
1	C	1934	GLN
1	C	2011	GLN
1	C	2019	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GY3	B	2240	-	25,25,25	3.45	10 (40%)	26,36,36	2.41	8 (30%)
2	GY3	A	3000	-	25,25,25	3.18	9 (36%)	26,36,36	2.68	9 (34%)
2	GY3	B	3000	-	25,25,25	3.15	8 (32%)	26,36,36	2.91	10 (38%)

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	GY3	B	2240	-	-	2/8/36/36	0/2/3/3
2	GY3	A	3000	-	-	0/8/36/36	0/2/3/3
2	GY3	B	3000	-	-	2/8/36/36	0/2/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	GY3	O12-C7	8.32	1.37	1.22
2	B	2240	GY3	N8-N4	-8.08	1.25	1.41
2	B	2240	GY3	O12-C7	8.07	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	GY3	N8-N4	-7.89	1.26	1.41
2	B	3000	GY3	O12-C7	7.75	1.36	1.22
2	B	3000	GY3	N8-N4	-7.74	1.26	1.41
2	B	2240	GY3	C19-C6	-6.45	1.39	1.52
2	B	3000	GY3	C19-C6	-6.08	1.40	1.52
2	B	2240	GY3	C24-C25	5.81	1.57	1.48
2	A	3000	GY3	C19-C6	-5.58	1.41	1.52
2	B	2240	GY3	O1-C2	4.89	1.47	1.43
2	B	3000	GY3	C24-C25	4.89	1.55	1.48
2	A	3000	GY3	O1-C2	4.32	1.46	1.43
2	A	3000	GY3	C24-C25	4.27	1.54	1.48
2	B	3000	GY3	C26-C25	4.23	1.55	1.29
2	B	2240	GY3	C26-C25	4.19	1.55	1.29
2	A	3000	GY3	C26-C25	4.06	1.54	1.29
2	B	2240	GY3	C6-C7	-3.46	1.37	1.52
2	B	3000	GY3	C6-C7	-3.40	1.37	1.52
2	B	2240	GY3	C6-C5	-3.31	1.38	1.52
2	B	3000	GY3	O1-C2	3.28	1.45	1.43
2	A	3000	GY3	C6-C7	-3.18	1.38	1.52
2	A	3000	GY3	C6-C5	-3.12	1.39	1.52
2	B	3000	GY3	C6-C5	-3.08	1.39	1.52
2	A	3000	GY3	C9-N8	2.38	1.49	1.46
2	B	2240	GY3	C9-N8	2.32	1.49	1.46
2	B	2240	GY3	C9-C10	2.17	1.53	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	GY3	C24-C25-C26	-8.14	112.59	126.20
2	B	3000	GY3	C24-C25-C26	-7.24	114.09	126.20
2	B	2240	GY3	C24-C25-C26	-6.62	115.13	126.20
2	B	3000	GY3	C10-O1-C2	-5.86	108.12	114.09
2	B	3000	GY3	C9-N8-C7	-5.24	116.22	127.62
2	B	3000	GY3	C3-N4-C5	-5.04	116.65	127.62
2	B	3000	GY3	C9-N8-N4	4.64	133.68	119.27
2	A	3000	GY3	C10-O1-C2	-4.54	109.46	114.09
2	A	3000	GY3	C9-N8-C7	-4.37	118.11	127.62
2	B	3000	GY3	C3-N4-N8	4.29	132.60	119.27
2	A	3000	GY3	C9-N8-N4	4.20	132.31	119.27
2	B	2240	GY3	C10-O1-C2	-4.04	109.97	114.09
2	B	2240	GY3	C3-N4-C5	-4.03	118.85	127.62
2	A	3000	GY3	C3-N4-C5	-3.86	119.21	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2240	GY3	C9-N8-C7	-3.82	119.30	127.62
2	B	2240	GY3	C3-N4-N8	3.76	130.96	119.27
2	A	3000	GY3	C3-N4-N8	3.62	130.51	119.27
2	B	2240	GY3	C9-N8-N4	3.57	130.37	119.27
2	B	3000	GY3	C23-C24-C25	-2.47	117.12	120.25
2	B	2240	GY3	C19-C6-C5	2.38	129.11	115.49
2	A	3000	GY3	C19-C6-C5	2.36	129.00	115.49
2	B	3000	GY3	C19-C6-C5	2.36	128.97	115.49
2	B	3000	GY3	C23-C22-C21	2.27	120.64	118.11
2	A	3000	GY3	C23-C24-C25	-2.16	117.52	120.25
2	B	2240	GY3	C19-C24-C25	2.14	124.33	121.64
2	B	3000	GY3	C19-C24-C25	2.07	124.24	121.64
2	A	3000	GY3	C19-C6-C7	2.00	126.95	115.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3000	GY3	C19-C24-C25-C26
2	B	3000	GY3	C23-C24-C25-C26
2	B	2240	GY3	C19-C24-C25-C26
2	B	2240	GY3	C23-C24-C25-C26

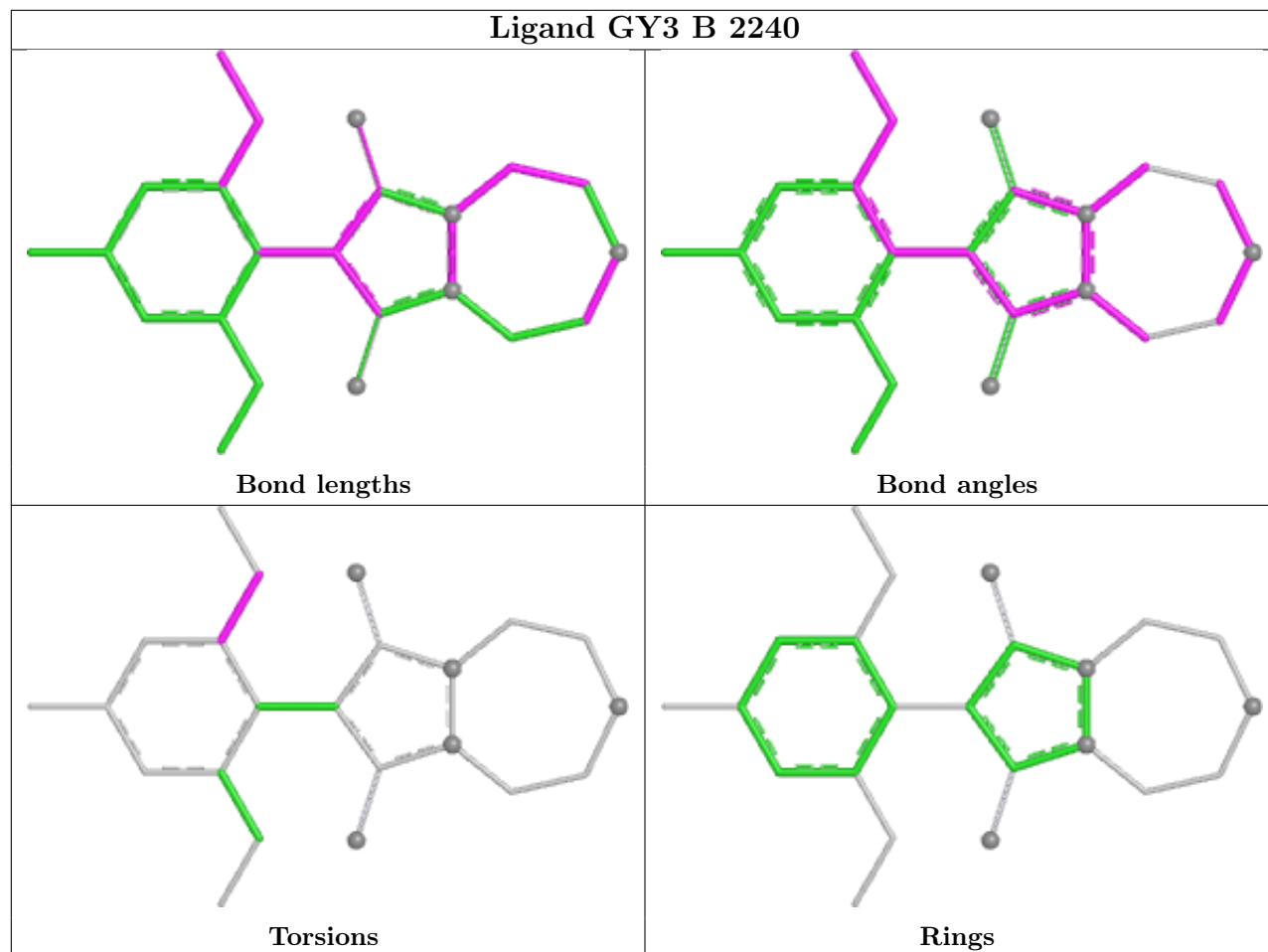
There are no ring outliers.

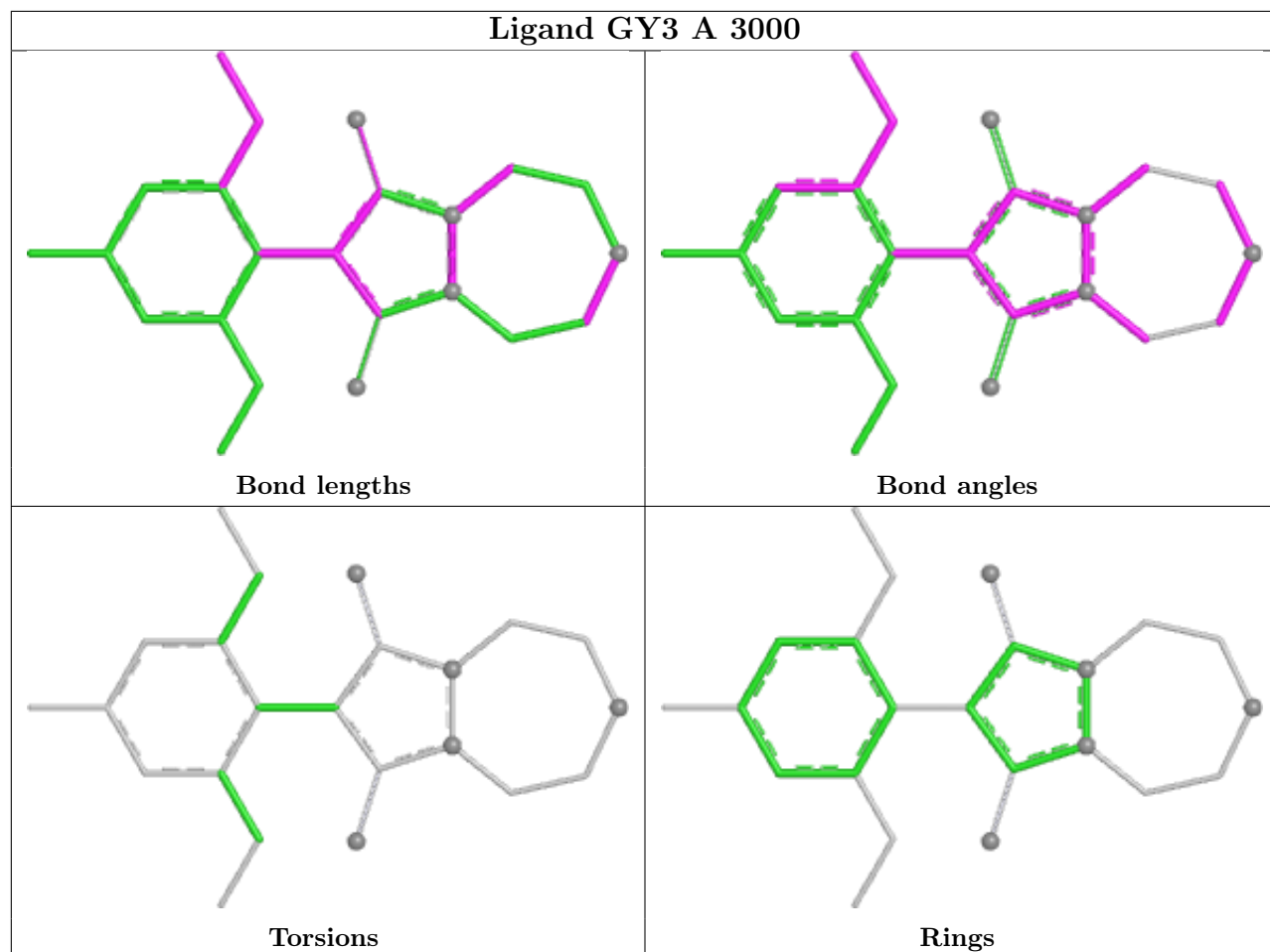
3 monomers are involved in 25 short contacts:

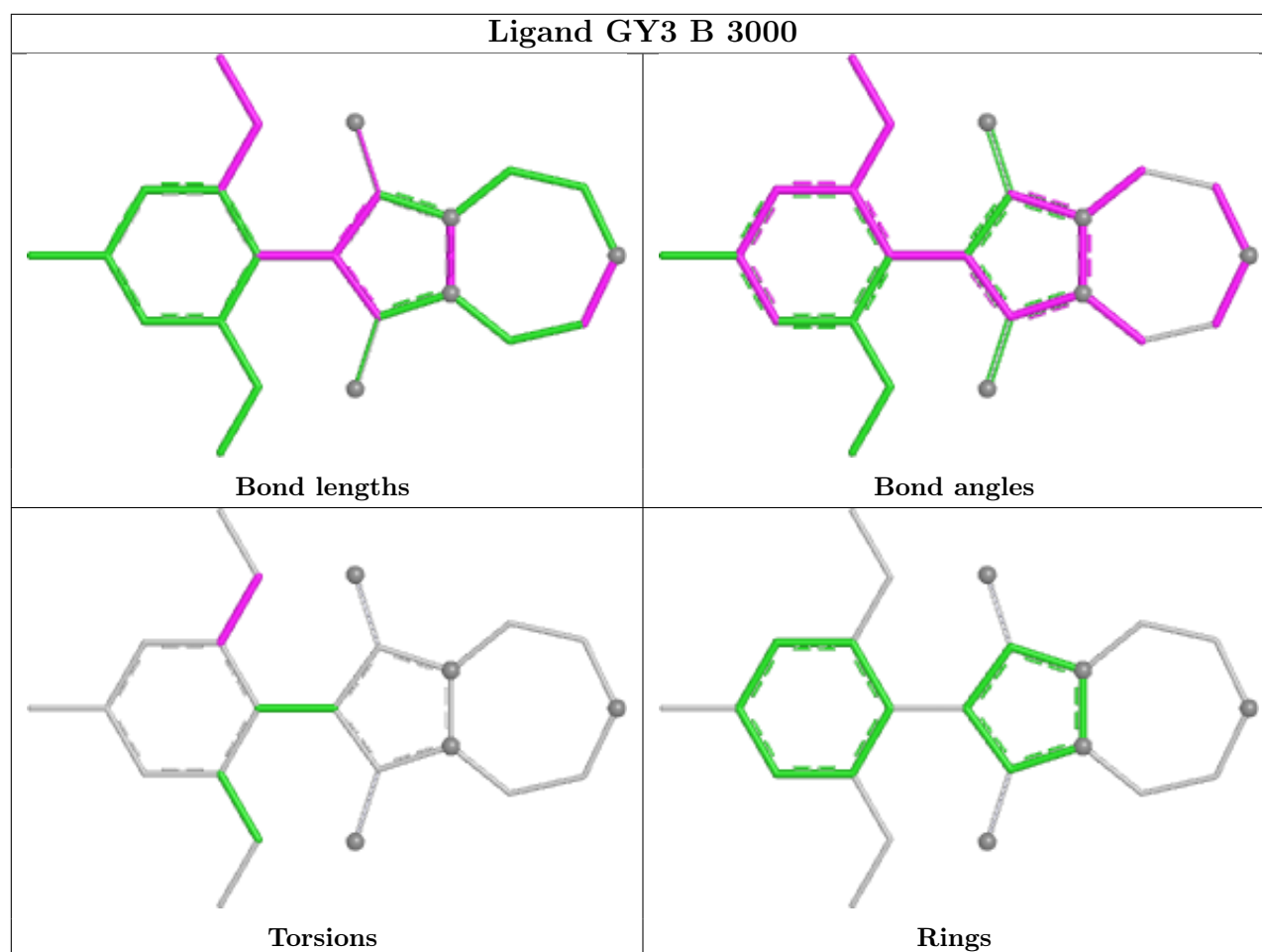
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2240	GY3	20	0
2	A	3000	GY3	1	0
2	B	3000	GY3	4	0

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	688/764 (90%)	-0.08	23 (3%)	46 36	50, 85, 192, 257	0
1	B	680/764 (89%)	0.06	35 (5%)	28 19	49, 95, 221, 292	0
1	C	675/764 (88%)	0.02	33 (4%)	29 20	49, 96, 227, 314	0
All	All	2043/2292 (89%)	-0.00	91 (4%)	33 23	49, 92, 216, 314	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	8.5
1	B	1685	GLU	7.9
1	B	2191	LEU	7.1
1	A	1685	GLU	5.6
1	B	2144	GLY	5.2
1	C	1681	VAL	5.1
1	B	2143	VAL	5.0
1	A	2144	GLY	4.8
1	B	1481	ARG	4.6
1	A	2143	VAL	4.5
1	C	2037	ARG	4.4
1	A	2080	ARG	4.2
1	B	1838	ASP	4.2
1	B	1684	GLY	4.1
1	A	1838	ASP	4.0
1	C	1679	ARG	4.0
1	C	1680	THR	3.8
1	B	2145	GLU	3.7
1	C	1910	PRO	3.6
1	B	1839	GLU	3.6
1	A	1483	ILE	3.6
1	B	2037	ARG	3.6
1	C	2051	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	2146	ALA	3.5
1	A	1480	LEU	3.4
1	C	1646	ALA	3.3
1	B	2084	PRO	3.3
1	B	1480	LEU	3.2
1	B	2044	MET	3.2
1	A	1481	ARG	3.1
1	B	1679	ARG	3.1
1	B	2082	LEU	3.0
1	A	1680	THR	3.0
1	C	2144	GLY	3.0
1	C	1648	ASN	2.9
1	C	1838	ASP	2.9
1	B	1681	VAL	2.9
1	A	1482	PRO	2.8
1	A	1647	ALA	2.8
1	C	1649	PRO	2.8
1	A	1682	ILE	2.8
1	A	1839	GLU	2.7
1	C	1685	GLU	2.7
1	A	1529	ASP	2.7
1	C	1682	ILE	2.7
1	B	2041	LEU	2.7
1	B	1824	LYS	2.6
1	A	1678	GLU	2.6
1	B	1649	PRO	2.6
1	C	1640	GLN	2.5
1	B	1648	ASN	2.5
1	C	1650	ASP	2.5
1	B	2086	TYR	2.5
1	B	1640	GLN	2.5
1	A	1683	ASN	2.4
1	B	2083	LEU	2.4
1	B	1680	THR	2.4
1	B	1486	PRO	2.4
1	C	1669	PHE	2.4
1	C	1911	ASN	2.4
1	C	2191	LEU	2.4
1	B	2085	ILE	2.4
1	B	1639	PHE	2.3
1	A	1681	VAL	2.3
1	C	2141	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2190	LYS	2.3
1	C	1668	LYS	2.3
1	B	2036	ARG	2.3
1	C	1546	GLU	2.3
1	C	2193	SER	2.3
1	B	1772	THR	2.2
1	C	1683	ASN	2.2
1	A	1527	SER	2.2
1	C	1647	ALA	2.2
1	A	1910	PRO	2.2
1	B	1769	GLU	2.2
1	C	1673	ASN	2.2
1	C	1674	SER	2.2
1	C	1726	THR	2.2
1	C	2192	GLU	2.1
1	A	1679	ARG	2.1
1	A	1546	GLU	2.1
1	B	1641	VAL	2.1
1	B	1656	LEU	2.1
1	A	1530	VAL	2.1
1	B	1794	VAL	2.1
1	C	1666	LEU	2.0
1	C	1639	PHE	2.0
1	C	1641	VAL	2.0
1	A	1526	PHE	2.0
1	C	1840	THR	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](#)

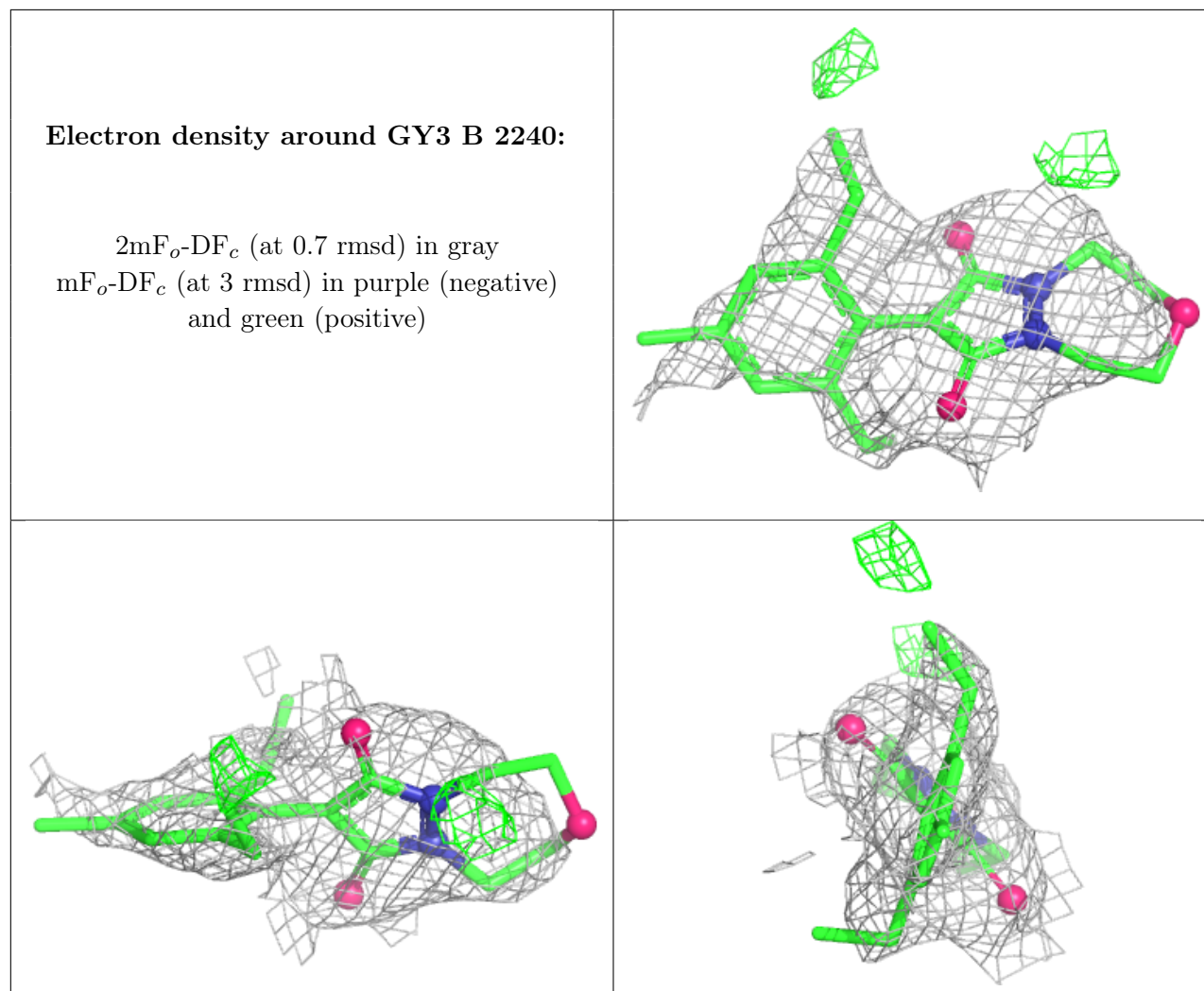
There are no monosaccharides in this entry.

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.

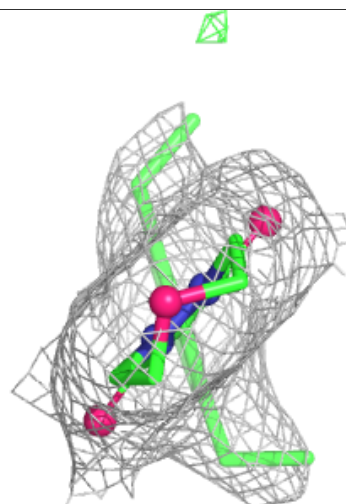
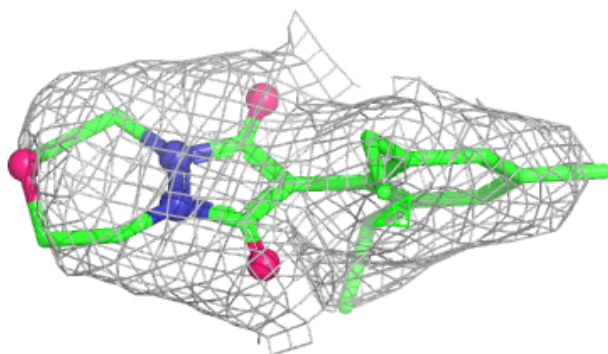
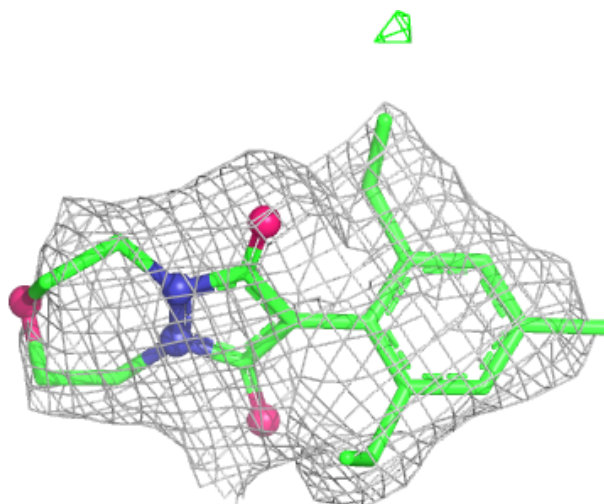
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GY3	B	2240	23/23	0.86	0.30	139,156,186,191	0
2	GY3	B	3000	23/23	0.94	0.26	104,116,138,147	0
2	GY3	A	3000	23/23	0.95	0.16	59,66,79,86	0

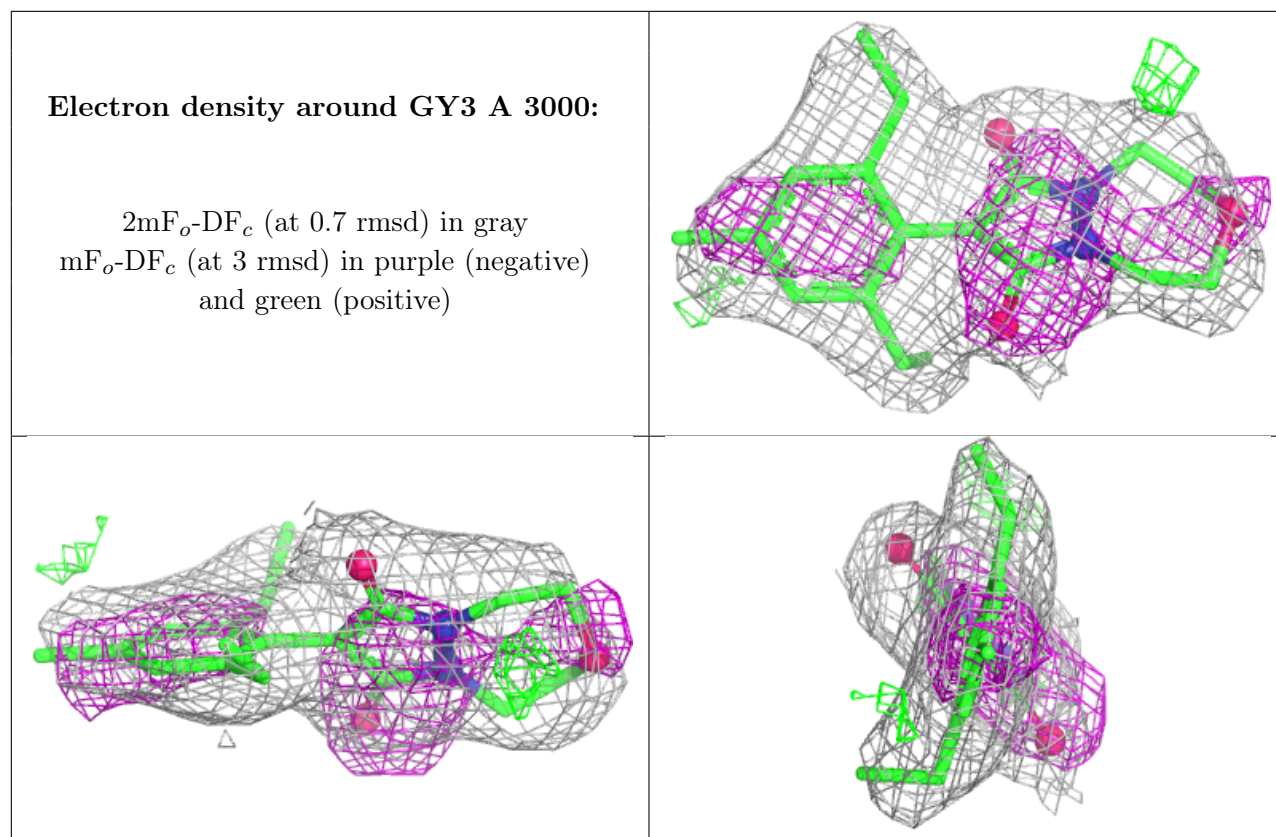
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around GY3 B 3000:

$2mF_o-DF_c$ (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.