



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 3PGQ / pdb_00003pgq
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

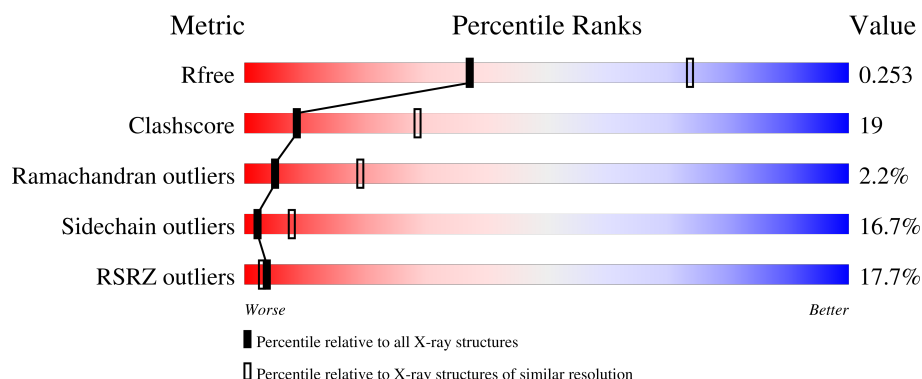
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	764	13% 56% 26% 6% 10%
1	B	764	18% 54% 26% 8% 11%
1	C	764	17% 54% 28% 6% 12%

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](#)

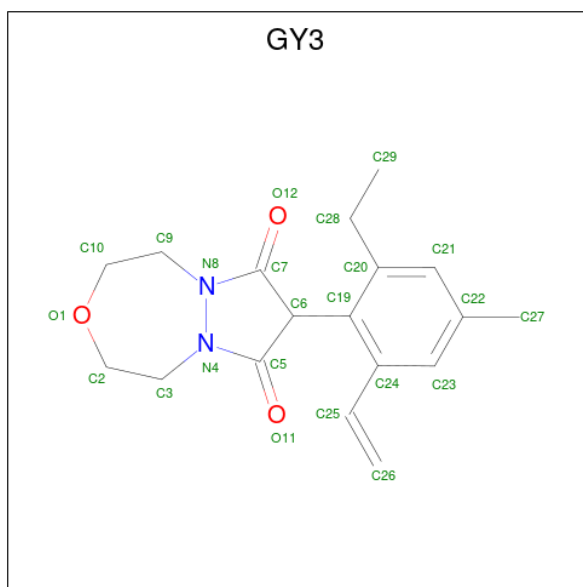
There are 2 unique types of molecules in this entry. The entry contains 16368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: GY3) (formula: C₁₈H₂₂N₂O₃).

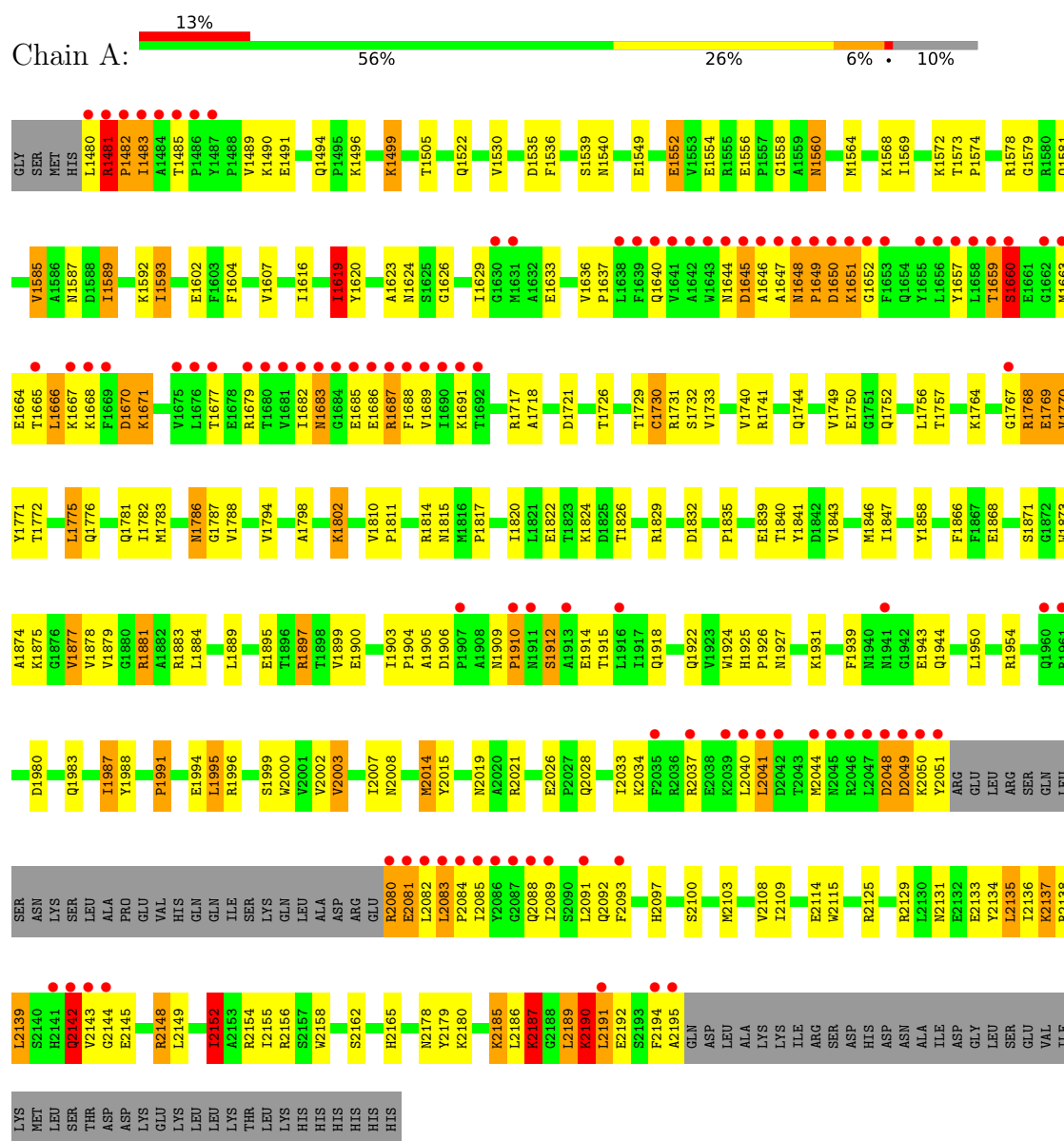


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	18	2	3		
2	B	1	Total	C	N	O	0	0
			23	18	2	3		
2	B	1	Total	C	N	O	0	0
			23	18	2	3		

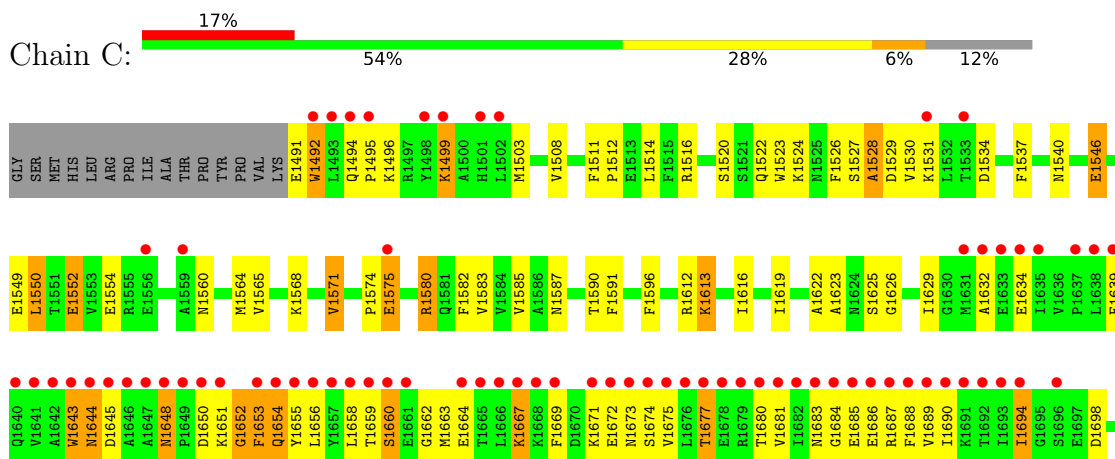
3 Residue-property plots

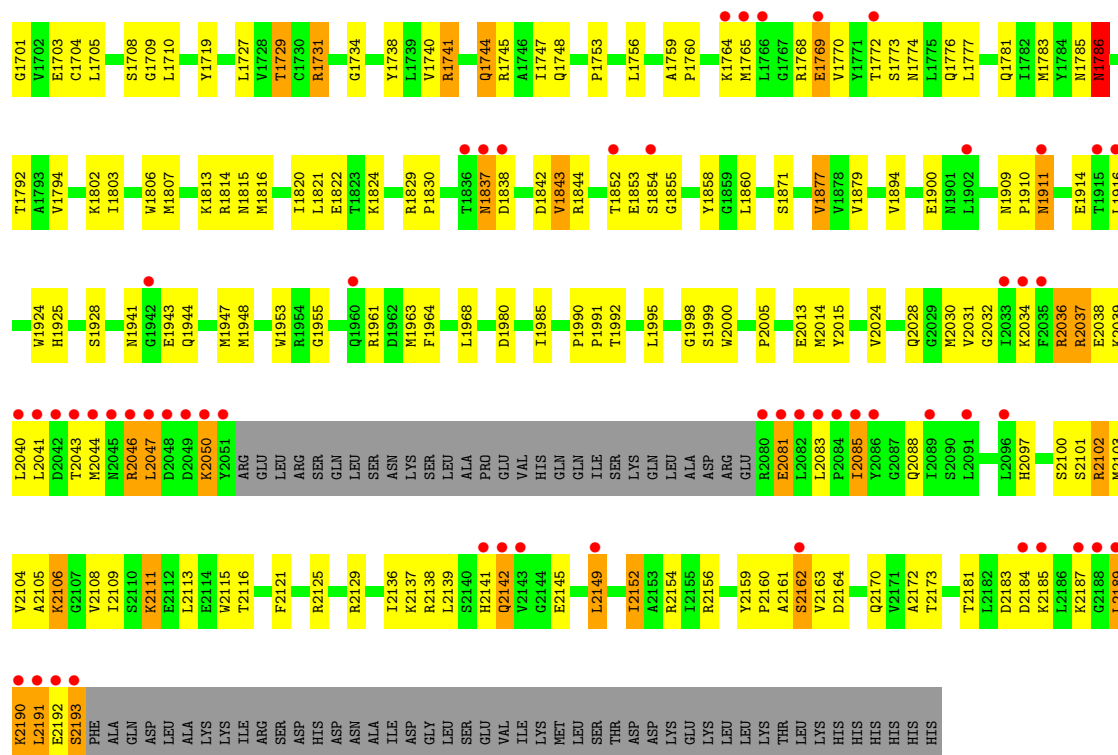
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Acetyl-CoA carboxylase



• Molecule 1: Acetyl-CoA carboxylase





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 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.80) 98.3 (30.00-2.80)	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 , 0.253	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 , 60.2	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	0.76	0/5614	0.96	11/7605 (0.1%)
1	B	0.75	0/5542	1.06	15/7509 (0.2%)
1	C	0.74	0/5505	0.92	12/7454 (0.2%)
All	All	0.75	0/16661	0.98	38/22568 (0.2%)

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 (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1481	ARG	CA-C-N	23.52	149.24	119.84
1	B	1481	ARG	C-N-CA	23.52	149.24	119.84
1	B	1481	ARG	O-C-N	-22.55	95.38	121.32
1	B	1482	PRO	CA-C-N	11.96	143.50	121.97
1	B	1482	PRO	C-N-CA	11.96	143.50	121.97
1	B	1481	ARG	CB-CA-C	10.68	131.20	110.17
1	A	1483	ILE	N-CA-C	9.44	120.25	110.72
1	C	1837	ASN	CB-CA-C	7.39	125.12	110.42
1	A	1939	PHE	N-CA-C	-7.32	103.00	112.23
1	C	2162	SER	N-CA-C	-6.60	105.52	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1991	PRO	CA-C-N	-6.48	112.30	122.73
1	A	1991	PRO	C-N-CA	-6.48	112.30	122.73
1	C	1729	THR	N-CA-C	-6.45	106.04	114.04
1	B	2125	ARG	N-CA-C	-6.42	104.20	111.14
1	B	1481	ARG	C-N-CD	-6.32	99.09	125.00
1	B	1691	LYS	N-CA-C	-6.29	106.20	114.31
1	A	1691	LYS	N-CA-C	-6.27	106.26	114.04
1	C	1941	ASN	N-CA-C	6.12	119.22	111.69
1	C	2102	ARG	N-CA-C	-5.96	104.69	111.07
1	C	1837	ASN	CA-C-N	5.87	131.74	121.52
1	C	1837	ASN	C-N-CA	5.87	131.74	121.52
1	B	1556	GLU	CA-C-N	-5.70	113.91	119.90
1	B	1556	GLU	C-N-CA	-5.70	113.91	119.90
1	B	1927	ASN	N-CA-C	5.43	116.88	111.07
1	B	1991	PRO	CA-C-N	-5.43	113.98	122.73
1	B	1991	PRO	C-N-CA	-5.43	113.98	122.73
1	C	1837	ASN	N-CA-C	5.39	122.29	110.80
1	A	1485	THR	CA-C-N	5.34	124.67	118.85
1	A	1485	THR	C-N-CA	5.34	124.67	118.85
1	C	1877	VAL	CB-CA-C	-5.26	104.02	111.38
1	C	1843	VAL	CB-CA-C	-5.25	105.17	112.04
1	A	1491	GLU	N-CA-C	-5.23	106.74	113.02
1	C	1785	ASN	N-CA-C	5.19	117.68	111.71
1	C	1786	ASN	CB-CA-C	-5.15	102.10	110.85
1	A	1927	ASN	N-CA-C	5.13	116.56	111.07
1	A	1877	VAL	CB-CA-C	-5.10	104.23	111.38
1	B	2005	PRO	N-CA-C	-5.05	107.45	114.27
1	A	1619	ILE	CB-CA-C	-5.01	104.69	110.91

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	170	1
1	B	5421	0	5369	248	0
1	C	5387	0	5318	227	0
2	A	23	0	21	1	0
2	B	46	0	42	25	0
All	All	16368	0	16181	613	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 19.

All (613) 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:C:1860:LEU:CD2	1:C:1948:MET:HE1	1.91	1.00
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.25	0.99
1:B:2000:TRP:CH2	1:B:2014:MET:HE3	1.98	0.97
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
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:2005:PRO:HD3	1:C:2014:MET:HE3	1.50	0.91
1:C:2081:GLU:OE2	1:C:2081:GLU:HA	1.67	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2000:TRP:CZ2	1:B:2014:MET:HE3	2.08	0.88
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:B:2001:VAL:HG11	2:B:2240:GY3:H27	1.59	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: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:2189:LEU:HD13	1:B:2189:LEU:C	2.07	0.79
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:C:1546:GLU:CD	1:C:1546:GLU:H	1.92	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
1:C:1860:LEU:HD21	1:C:1948:MET:HE1	1.66	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:1963:MET:HE3	1:C:1783:MET:CE	2.16	0.75
1:B:1675:VAL:HG23	1:B:1677:THR:CG2	2.15	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1860:LEU:HD23	1:C:1948:MET:HE1	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: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:A:1682:ILE:O	1:A:1683:ASN:C	2.32	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:C:2005:PRO:CD	1:C:2014:MET:HE3	2.22	0.69
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:C:2081:GLU:OE2	1:C:2081:GLU:CA	2.42	0.68
1:A:1663:MET:HE2	1:A:1688:PHE:CD2	2.28	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:1562:ILE:HD11	1:B:1599:GLN:CD	2.19	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:A:2000:TRP:CD1	1:A:2000:TRP:C	2.73	0.67
1:B:2014:MET:HG2	1:B:2109:ILE:HG22	1.75	0.67
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:2189:LEU:C	1:B:2189:LEU:CD1	2.69	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2000:TRP:CE2	1:B:2014:MET:HE1	2.31	0.66
1:C:1663:MET:HE3	1:C:1688:PHE:CB	2.25	0.65
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: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: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:C	1:C:1909:ASN:HD22	2.06	0.62
1:C:1909:ASN:HD22	1:C:1911:ASN:H	1.47	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
1:C:1653:PHE:H	1:C:1653:PHE:HD2	1.47	0.62
1:C:1663:MET:HE3	1:C:1688:PHE:CG	2.34	0.62
1:B:2000:TRP:CE2	1:B:2014:MET:CE	2.82	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1673:ASN:H	1:B:1673:ASN:ND2	1.85	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:B:1996:ARG:O	1:B:1997:GLY:C	2.43	0.60
1:C:1523:TRP:CE2	1:C:1574:PRO:HD3	2.36	0.60
1:B:2001:VAL:HG11	2:B:2240:GY3:C27	2.28	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:C:1582:PHE:CD2	1:C:1807:MET:HE1	2.36	0.60
1:A:2133:GLU:OE1	1:A:2148:ARG:NH2	2.35	0.60
1:A:1564:MET:HE3	1:A:1604:PHE:HB2	1.83	0.59
1:A:1922:GLN:CD	1:A:1954:ARG:HH12	2.10	0.59
1:B:1846:MET:HE1	1:B:1990:PRO:HB2	1.82	0.59
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:C:2189:LEU:C	1:C:2191:LEU:H	2.10	0.59
1:A:1772:THR:H	1:A:1776:GLN:NE2	2.00	0.59
1:B:1663:MET:HE2	1:B:1688:PHE:CD1	2.38	0.58
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: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: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: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
1:B:1650:ASP:C	1:B:1652:GLY:N	2.62	0.57
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:A:1560:ASN:H	1:A:1560:ASN:ND2	1.88	0.57
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2001:VAL:CG1	2:B:2240:GY3:H27	2.32	0.56
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: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:1922:GLN:CD	1:A:1954:ARG:NH1	2.64	0.55
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.89	0.55
1:C:2041:LEU:CD2	1:C:2044:MET:HE1	2.37	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
2:B:2240:GY3:H27B	1:C:1738:TYR:CD1	2.41	0.55
1:B:2001:VAL:CG1	2:B:2240:GY3:C27	2.85	0.55
1:B:2189:LEU:C	1:B:2191:LEU:H	2.15	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:B:1947:MET:HE2	1:B:1985:ILE:HG12	1.89	0.54
1:A:2083:LEU:N	1:A:2084:PRO:HD2	2.23	0.54
1:B:1925:HIS:O	1:B:1926:PRO:C	2.51	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:B:1963:MET:HE3	1:C:1783:MET:HE2	1.88	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:C:2191:LEU:C	1:C:2193:SER:HB2	2.32	0.53
1:A:1798:ALA:O	1:A:1802:LYS:HD3	2.08	0.53
1:B:2147:SER:O	1:B:2148:ARG:C	2.51	0.53
1:A:1889:LEU:N	1:A:1889:LEU:HD23	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1566:ALA:HA	1:B:1584:VAL:O	2.09	0.53
1:C:1860:LEU:HD23	1:C:1948:MET:CE	2.38	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:A:2137:LYS:O	1:A:2138:ARG:C	2.50	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:B:1638:LEU:C	1:B:1638:LEU:HD12	2.34	0.52
1:A:1909:ASN:O	1:A:1910:PRO:C	2.52	0.52
1:B:1537:PHE:CD1	1:B:1537:PHE:C	2.88	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:A:1909:ASN:C	1:A:1909:ASN:OD1	2.52	0.51
1:B:2114:GLU:O	1:B:2115:TRP:C	2.53	0.51
1:B:2154:ARG:O	1:B:2157:SER:OG	2.27	0.51
1:C:1639:PHE:CD1	1:C:1639:PHE:C	2.88	0.51
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:A:1925:HIS:O	1:A:1926:PRO:C	2.53	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2044:MET:O	1:B:2047:LEU:C	2.54	0.51
1:C:2164:ASP:C	1:C:2164:ASP:OD1	2.54	0.51
1:B:2022:ALA:HB3	1:B:2103:MET:HE2	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:1591:PHE:C	1:C:1591:PHE:CD2	2.89	0.50
1:C:1852:THR:HB	1:C:1855:GLY:O	2.11	0.50
1:B:1513:GLU:HA	1:B:1513:GLU:OE2	2.10	0.50
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:1663:MET:HE3	1:C:1688:PHE:HB3	1.93	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:1659:THR:O	1:B:1660:SER:C	2.55	0.50
1:C:1659:THR:O	1:C:1660:SER:C	2.55	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:B:1511:PHE:O	1:B:1512:PRO:C	2.53	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:A:2008:ASN:C	1:A:2008:ASN:HD22	2.20	0.49
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:C:1701:GLY:O	1:C:1704:CYS:HB2	2.12	0.49
1:C:2100:SER:HA	1:C:2103:MET:HE3	1.93	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:C:2000:TRP:CD1	1:C:2000:TRP:C	2.91	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:A:1645:ASP:OD2	1:A:1645:ASP:C	2.56	0.49
1:A:2178:ASN:O	1:A:2179:TYR:C	2.55	0.49
1:C:1852:THR:CG2	1:C:1853:GLU:H	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2160:PRO:C	1:C:2162:SER:H	2.20	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:A:1922:GLN:OE1	1:A:1954:ARG:NH1	2.46	0.48
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.29	0.48
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:A:1664:GLU:O	1:A:1665:THR:C	2.55	0.48
1:A:1749:VAL:O	1:A:1750:GLU:C	2.57	0.48
1:B:1797:LEU:HD22	1:B:1801:GLU:HG3	1.94	0.48
1:A:1592:LYS:C	1:A:1593:ILE:HG12	2.37	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:1527:SER:C	1:C:1529:ASP:N	2.71	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:1527:SER:C	1:C:1529:ASP:H	2.21	0.48
1:C:1643:TRP:H	1:C:1643:TRP:CD1	2.31	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:C:2121:PHE:CD2	1:C:2121:PHE:C	2.91	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:B:1759:ALA:O	1:B:1760:PRO:C	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2040:LEU:C	1:C:2043:THR:HG22	2.39	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: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:C:2032:GLY:O	1:C:2036:ARG:HD2	2.14	0.47
1:A:2040:LEU:O	1:A:2041:LEU:C	2.57	0.47
1:B:1624:ASN:HD22	1:B:1626:GLY:N	2.05	0.47
1:B:2082:LEU:C	1:B:2084:PRO:HD2	2.39	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
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:B:1963:MET:HE3	1:C:1783:MET:HE1	1.94	0.47
1:C:1491:GLU:O	1:C:1491:GLU:CG	2.44	0.47
1:A:1659:THR:O	1:A:1660:SER:C	2.57	0.47
1:B:1954:ARG:NH1	1:B:1994:GLU:OE1	2.48	0.47
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.23	0.47
1:C:1659:THR:O	1:C:1662:GLY:N	2.36	0.47
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.78	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:1649:PRO:O	1:A:1650:ASP:C	2.57	0.47
1:C:1622:ALA:O	1:C:1729:THR:HG22	2.14	0.47
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:C:1672:GLU:C	1:C:1674:SER:H	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2041:LEU:HD22	1:C:2044:MET:HE1	1.96	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:1650:ASP:C	1:B:1652:GLY:H	2.22	0.46
1:C:1759:ALA:N	1:C:1760:PRO:CD	2.78	0.46
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.14	0.46
1:B:1963:MET:O	1:B:1964:PHE:C	2.58	0.46
1:A:1573:THR:HB	1:A:1574:PRO:HD2	1.96	0.46
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.15	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: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:2000:TRP:CH2	1:B:2014:MET:CE	2.81	0.45
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.15	0.45
1:A:1480:LEU:HB3	1:A:1481:ARG:H	1.50	0.45
1:A:2082:LEU:C	1:A:2084:PRO:HD2	2.41	0.45
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:C:2104:VAL:O	1:C:2105:ALA:C	2.60	0.45
1:B:1734:GLY:HA3	2:B:3000:GY3:C7	2.46	0.45
1:A:2152:ILE:HD13	1:A:2152:ILE:HA	1.58	0.45
1:C:1947:MET:HE2	1:C:1985:ILE:HG12	1.99	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:1664:GLU:C	1:A:1666:LEU:N	2.73	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:B:2180:LYS:C	1:B:2182:LEU:N	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.17	0.44
1:B:1833:PHE:C	1:B:1833:PHE:CD2	2.94	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:B:2089:ILE:CG2	1:B:2090:SER:N	2.77	0.44
1:C:2190:LYS:O	1:C:2190:LYS:CG	2.65	0.44
1:A:1651:LYS:HD2	1:A:1651:LYS:C	2.43	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: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: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:N	1:A:1560:ASN:ND2	2.55	0.44
1:B:1524:LYS:HD2	1:B:1524:LYS:HA	1.72	0.44
1:B:1833:PHE:CD2	1:B:1833:PHE:O	2.71	0.44
1:C:2041:LEU:HA	1:C:2044:MET:HE3	2.00	0.44
1:A:1535:ASP:C	1:A:1535:ASP:OD2	2.60	0.44
1:A:1843:VAL:O	1:A:1847:ILE:HG13	2.18	0.44
1:A:1846:MET:HE3	1:A:2115:TRP:CH2	2.53	0.44
1:B:1998:GLY:HA2	2:B:2240:GY3:C21	2.47	0.44
1:A:1717:ARG:O	1:A:1718:ALA:C	2.58	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:1999:SER:O	1:B:2000:TRP:C	2.60	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:1730:CYS:O	1:A:1731:ARG:HB3	2.17	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2114:GLU:O	1:A:2115:TRP:C	2.61	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:A:1494:GLN:NE2	1:A:1558:GLY:HA3	2.34	0.43
1:B:1636:VAL:O	1:B:1637:PRO:C	2.62	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:A:1983:GLN:CD	1:A:1983:GLN:N	2.76	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
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:2192:GLU:N	1:C:2193:SER:CB	2.81	0.43
1:B:2046:ARG:C	1:B:2047:LEU:HD22	2.44	0.43
1:C:2013:GLU:CD	1:C:2125:ARG:HH21	2.26	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:C:1511:PHE:O	1:C:1512:PRO:C	2.62	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:C:2137:LYS:O	1:C:2138:ARG:C	2.61	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:2030:MET:HE3	1:C:2034:LYS:HB2	1.99	0.42
1:C:2152:ILE:H	1:C:2152:ILE:HG12	1.68	0.42
1:A:2134:TYR:HD2	1:A:2135:LEU:HD13	1.84	0.42
1:B:1631:MET:HG3	1:C:2030:MET:HE2	2.02	0.42
1:A:1782:ILE:HG22	1:A:1783:MET:HE2	2.01	0.42
1:B:1662:GLY:O	1:B:1663:MET:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:2149:LEU:H	1:C:2149:LEU:HG	1.43	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:B:1783:MET:CE	1:C:1963:MET:HE3	2.49	0.42
1:B:2006:THR:HG22	1:C:1709:GLY:C	2.45	0.42
1:A:1569:ILE:O	1:A:1581:GLN:HA	2.20	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
1:B:2106:LYS:NZ	1:C:1698:ASP:OD1	2.42	0.42
1:C:1527:SER:O	1:C:1528:ALA:C	2.63	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:1998:GLY:HA2	2:B:2240:GY3:C23	2.50	0.41
1:C:2183:ASP:O	1:C:2184:ASP:C	2.64	0.41
1:A:2189:LEU:O	1:A:2190:LYS:C	2.62	0.41
1:C:2046:ARG:HG3	1:C:2047:LEU:HD13	2.02	0.41
1:A:2100:SER:HA	1:A:2103:MET:HE3	2.02	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:1564:MET:HE1	1:C:1596:PHE:CE2	2.55	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:B:1685:GLU:O	1:B:1686:GLU:C	2.63	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:2134:TYR:CD2	1:A:2134:TYR:C	2.98	0.41
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.19	0.41
1:C:2041:LEU:HD23	1:C:2044:MET:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2044:MET:HE2	1:B:2044:MET:HB2	1.88	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:A:1841:TYR:CD1	1:A:1841:TYR:C	2.98	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:C:2160:PRO:C	1:C:2162:SER:N	2.79	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:1624:ASN:ND2	1:B:1624:ASN:C	2.79	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:B:2180:LYS:C	1:B:2182:LEU:H	2.28	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:C:1998:GLY:O	1:C:1999:SER:C	2.64	0.41
1:A:1644:ASN:OD1	1:A:1652:GLY:C	2.64	0.40
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:B:2082:LEU:C	1:B:2084:PRO:CD	2.93	0.40
1:C:1639:PHE:HA	1:C:1658:LEU:HD23	2.04	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2186:LEU:O	1:A:2187:LYS:C	2.64	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:C:2172:ALA:O	1:C:2173:THR:C	2.63	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: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:C:1511:PHE:O	1:C:1514:LEU:N	2.55	0.40
1:C:1612:ARG:O	1:C:1613:LYS:C	2.63	0.40
1:C:1837:ASN:OD1	1:C:1992:THR:HG22	2.21	0.40
1:C:2137:LYS:C	1:C:2139:LEU:N	2.76	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%)	5	19
1	B	676/764 (88%)	601 (89%)	55 (8%)	20 (3%)	3	12
1	C	671/764 (88%)	615 (92%)	46 (7%)	10 (2%)	8	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2031/2292 (89%)	1837 (90%)	149 (7%)	45 (2%)	5	19

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
1	A	1671	LYS
1	A	1910	PRO
1	B	1660	SER
1	B	1744	GLN
1	B	2190	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	487 (83%)	97 (17%)	2	8
1	B	577/654 (88%)	481 (83%)	96 (17%)	2	8
1	C	573/654 (88%)	476 (83%)	97 (17%)	2	7
All	All	1734/1962 (88%)	1444 (83%)	290 (17%)	2	8

All (290) 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
1	A	1554	GLU
1	A	1556	GLU
1	A	1560	ASN
1	A	1568	LYS
1	A	1578	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1585	VAL
1	A	1589	ILE
1	A	1593	ILE
1	A	1602	GLU
1	A	1616	ILE
1	A	1619	ILE
1	A	1629	ILE
1	A	1640	GLN
1	A	1645	ASP
1	A	1648	ASN
1	A	1651	LYS
1	A	1659	THR
1	A	1660	SER
1	A	1666	LEU
1	A	1668	LYS
1	A	1679	ARG
1	A	1685	GLU
1	A	1686	GLU
1	A	1687	ARG
1	A	1730	CYS
1	A	1732	SER
1	A	1757	THR
1	A	1764	LYS
1	A	1769	GLU
1	A	1770	VAL
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	1824	LYS
1	A	1826	THR
1	A	1839	GLU
1	A	1840	THR
1	A	1871	SER
1	A	1877	VAL
1	A	1878	VAL
1	A	1879	VAL
1	A	1881	ARG
1	A	1884	LEU
1	A	1897	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1900	GLU
1	A	1906	ASP
1	A	1914	GLU
1	A	1915	THR
1	A	1918	GLN
1	A	1924	TRP
1	A	1950	LEU
1	A	1980	ASP
1	A	1987	ILE
1	A	1995	LEU
1	A	1996	ARG
1	A	1999	SER
1	A	2002	VAL
1	A	2003	VAL
1	A	2014	MET
1	A	2026	GLU
1	A	2028	GLN
1	A	2037	ARG
1	A	2041	LEU
1	A	2044	MET
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	2135	LEU
1	A	2137	LYS
1	A	2139	LEU
1	A	2142	GLN
1	A	2145	GLU
1	A	2148	ARG
1	A	2149	LEU
1	A	2152	ILE
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	B	1480	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1481	ARG
1	B	1503	MET
1	B	1516	ARG
1	B	1524	LYS
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	1565	VAL
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	1613	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	1663	MET
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	1726	THR
1	B	1731	ARG
1	B	1757	THR
1	B	1769	GLU
1	B	1781	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1902	LEU
1	B	1911	ASN
1	B	1914	GLU
1	B	1915	THR
1	B	1917	ILE
1	B	1968	LEU
1	B	1980	ASP
1	B	1995	LEU
1	B	2001	VAL
1	B	2003	VAL
1	B	2006	THR
1	B	2011	GLN
1	B	2014	MET
1	B	2021	ARG
1	B	2034	LYS
1	B	2041	LEU
1	B	2043	THR
1	B	2044	MET
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	2113	LEU
1	B	2126	LEU
1	B	2127	ARG
1	B	2133	GLU
1	B	2137	LYS
1	B	2143	VAL
1	B	2145	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2173	THR
1	B	2180	LYS
1	B	2185	LYS
1	B	2189	LEU
1	B	2191	LEU
1	C	1499	LYS
1	C	1503	MET
1	C	1508	VAL
1	C	1516	ARG
1	C	1520	SER
1	C	1522	GLN
1	C	1524	LYS
1	C	1531	LYS
1	C	1534	ASP
1	C	1546	GLU
1	C	1549	GLU
1	C	1550	LEU
1	C	1552	GLU
1	C	1554	GLU
1	C	1565	VAL
1	C	1568	LYS
1	C	1571	VAL
1	C	1575	GLU
1	C	1580	ARG
1	C	1583	VAL
1	C	1585	VAL
1	C	1613	LYS
1	C	1616	ILE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1667	LYS
1	C	1677	THR
1	C	1680	THR
1	C	1685	GLU
1	C	1686	GLU
1	C	1687	ARG
1	C	1690	ILE
1	C	1694	ILE
1	C	1731	ARG
1	C	1740	VAL
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	1794	VAL
1	C	1802	LYS
1	C	1820	ILE
1	C	1822	GLU
1	C	1824	LYS
1	C	1838	ASP
1	C	1843	VAL
1	C	1871	SER
1	C	1877	VAL
1	C	1879	VAL
1	C	1900	GLU
1	C	1911	ASN
1	C	1914	GLU
1	C	1916	LEU
1	C	1924	TRP
1	C	1961	ARG
1	C	1968	LEU
1	C	1980	ASP
1	C	2028	GLN
1	C	2031	VAL
1	C	2036	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2037	ARG
1	C	2038	GLU
1	C	2039	LYS
1	C	2046	ARG
1	C	2047	LEU
1	C	2050	LYS
1	C	2081	GLU
1	C	2083	LEU
1	C	2085	ILE
1	C	2088	GLN
1	C	2101	SER
1	C	2106	LYS
1	C	2111	LYS
1	C	2116	THR
1	C	2129	ARG
1	C	2149	LEU
1	C	2152	ILE
1	C	2163	VAL
1	C	2181	THR
1	C	2185	LYS
1	C	2187	LYS
1	C	2189	LEU
1	C	2191	LEU
1	C	2193	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1517	GLN
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	1965	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2008	ASN
1	A	2092	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	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
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	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	1922	GLN
1	B	1925	HIS
1	B	1934	GLN
1	B	1944	GLN
1	B	2011	GLN
1	B	2088	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1909	ASN
1	C	1911	ASN
1	C	1922	GLN
1	C	1934	GLN
1	C	1983	GLN
1	C	2011	GLN
1	C	2019	ASN
1	C	2045	ASN
1	C	2170	GLN

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](#)

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
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
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 26 short contacts:

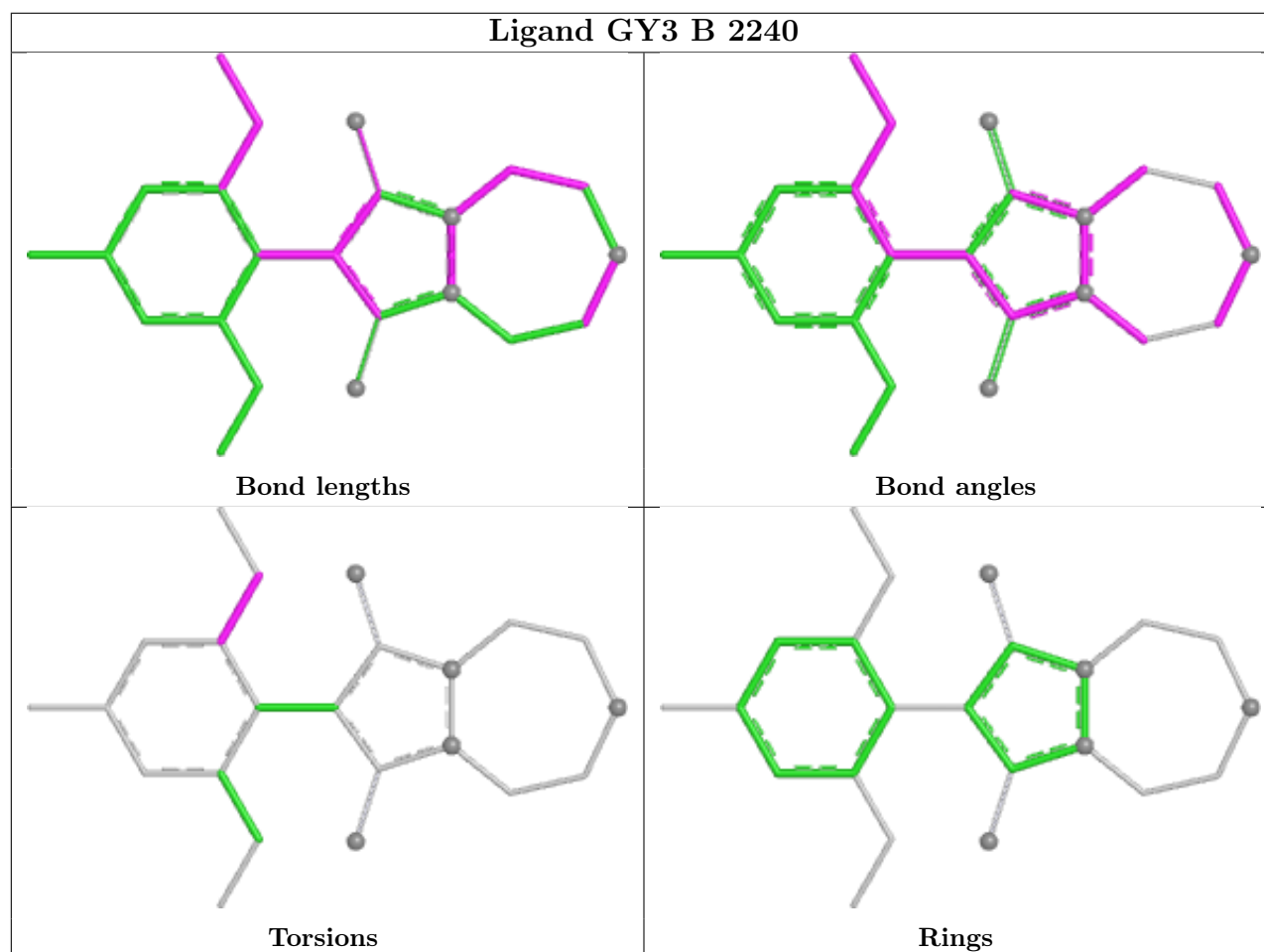
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2240	GY3	21	0

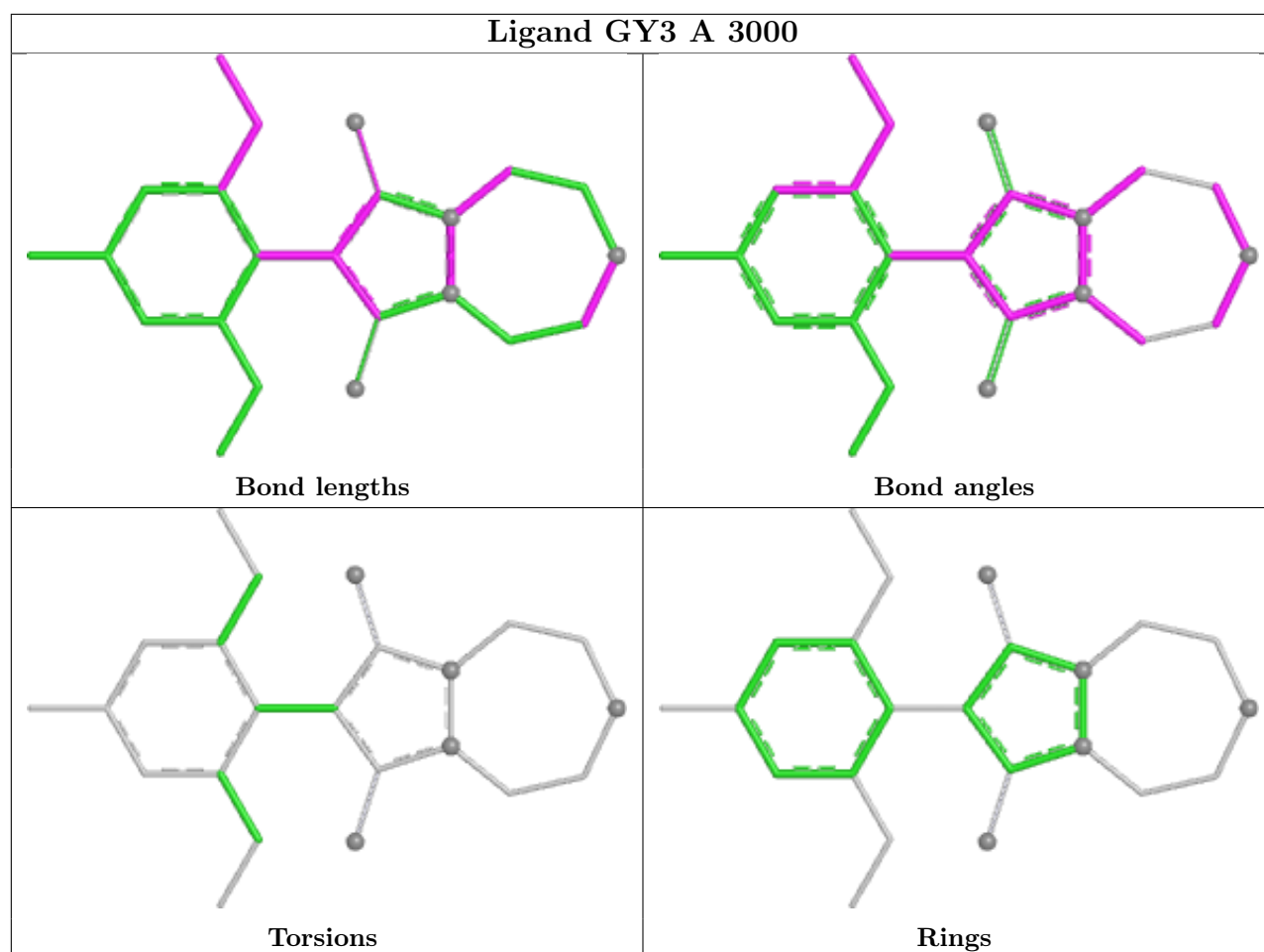
Continued on next page...

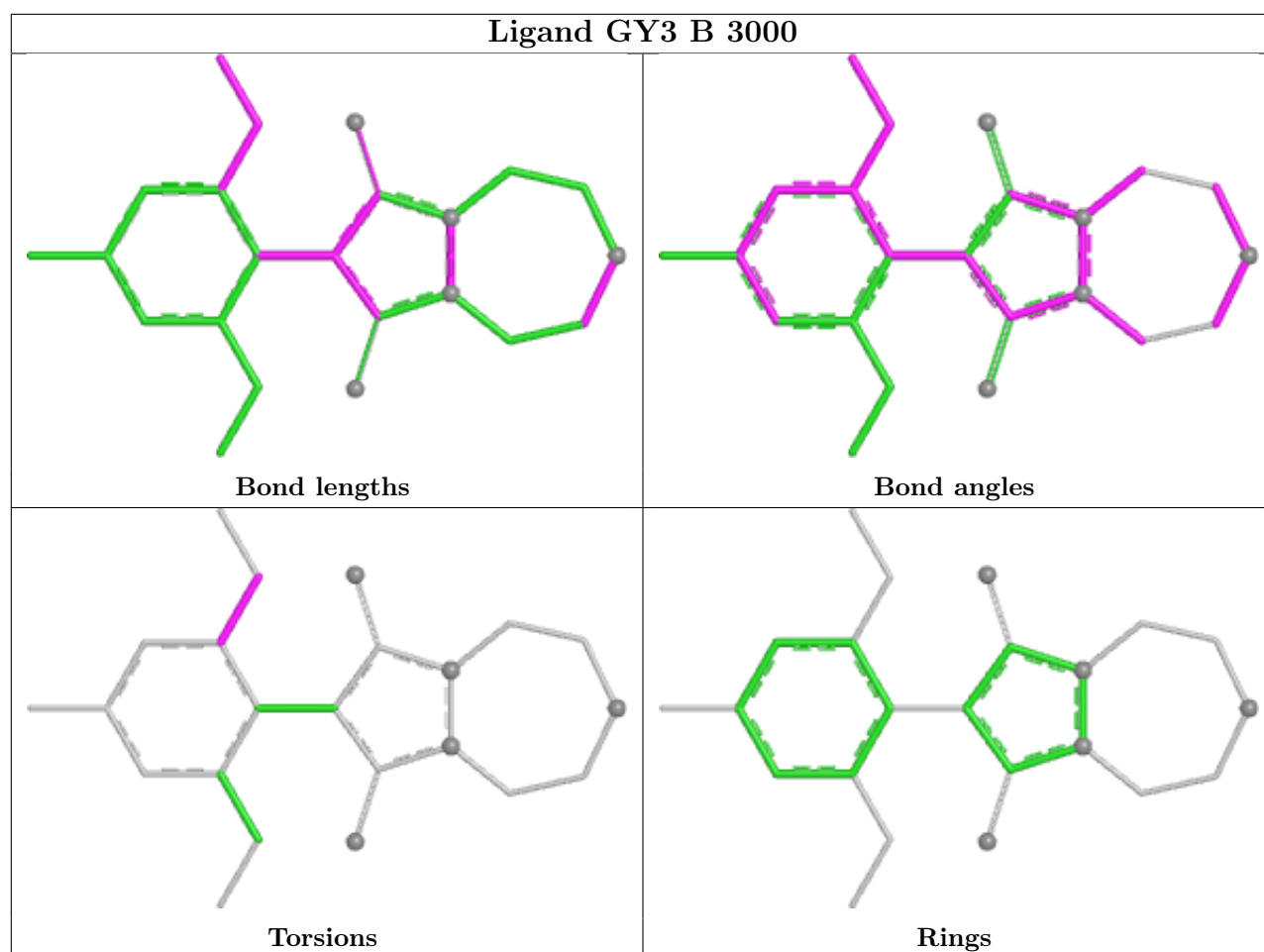
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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%)	0.65	97 (14%) 6 5	50, 85, 192, 257	0
1	B	680/764 (89%)	0.97	137 (20%) 3 2	49, 95, 221, 292	0
1	C	675/764 (88%)	0.97	128 (18%) 3 2	49, 96, 227, 314	0
All	All	2043/2292 (89%)	0.86	362 (17%) 4 3	49, 92, 216, 314	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2051	TYR	8.7
1	A	2051	TYR	7.9
1	B	2047	LEU	7.7
1	A	1482	PRO	7.5
1	B	1481	ARG	7.2
1	A	1684	GLY	7.2
1	C	1680	THR	7.0
1	B	1682	ILE	6.9
1	C	1645	ASP	6.7
1	B	1683	ASN	6.7
1	C	1674	SER	6.6
1	B	1483	ILE	6.5
1	B	1482	PRO	6.4
1	A	1643	TRP	6.3
1	A	2050	LYS	6.2
1	C	2045	ASN	6.2
1	C	2082	LEU	6.2
1	C	2083	LEU	6.2
1	C	2050	LYS	6.1
1	B	2144	GLY	6.0
1	A	1681	VAL	5.8
1	A	1647	ALA	5.7
1	B	1655	TYR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1650	ASP	5.6
1	A	2195	ALA	5.6
1	C	2143	VAL	5.6
1	B	1684	GLY	5.6
1	A	1649	PRO	5.5
1	B	1643	TRP	5.4
1	C	2080	ARG	5.4
1	A	2143	VAL	5.3
1	A	1660	SER	5.3
1	B	1680	THR	5.3
1	B	1653	PHE	5.3
1	B	1480	LEU	5.2
1	B	1651	LYS	5.2
1	B	2190	LYS	5.1
1	C	1687	ARG	5.1
1	C	1655	TYR	5.1
1	C	1673	ASN	5.0
1	A	1655	TYR	5.0
1	C	1681	VAL	5.0
1	A	2047	LEU	5.0
1	B	2081	GLU	5.0
1	B	2045	ASN	5.0
1	B	1644	ASN	4.9
1	A	1680	THR	4.9
1	C	1686	GLU	4.9
1	C	1679	ARG	4.8
1	B	2086	TYR	4.8
1	B	2083	LEU	4.8
1	B	1647	ALA	4.7
1	B	2041	LEU	4.7
1	C	2084	PRO	4.7
1	B	1642	ALA	4.6
1	C	1684	GLY	4.6
1	C	1492	TRP	4.6
1	B	2181	THR	4.6
1	B	2082	LEU	4.6
1	A	2080	ARG	4.6
1	B	2191	LEU	4.5
1	C	1638	LEU	4.5
1	C	1660	SER	4.5
1	B	1687	ARG	4.5
1	B	1686	GLU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1646	ALA	4.5
1	B	1637	PRO	4.4
1	A	1640	GLN	4.4
1	C	2081	GLU	4.4
1	B	2085	ILE	4.4
1	A	1641	VAL	4.4
1	B	2143	VAL	4.4
1	A	2045	ASN	4.4
1	C	1647	ALA	4.4
1	A	2081	GLU	4.4
1	B	1660	SER	4.3
1	C	2041	LEU	4.3
1	C	1837	ASN	4.3
1	A	1483	ILE	4.3
1	B	1641	VAL	4.3
1	C	1666	LEU	4.3
1	A	1659	THR	4.3
1	C	1683	ASN	4.3
1	C	1765	MET	4.2
1	A	1682	ILE	4.2
1	A	1910	PRO	4.2
1	B	1689	VAL	4.1
1	A	2082	LEU	4.1
1	B	1638	LEU	4.1
1	C	1641	VAL	4.1
1	C	2193	SER	4.1
1	A	2144	GLY	4.1
1	C	1682	ILE	4.1
1	C	2048	ASP	4.1
1	B	1688	PHE	4.1
1	C	1676	LEU	4.0
1	A	2194	PHE	4.0
1	B	2043	THR	4.0
1	B	1645	ASP	4.0
1	B	1649	PRO	4.0
1	B	2162	SER	4.0
1	A	1651	LYS	4.0
1	B	2046	ARG	4.0
1	B	1646	ALA	3.9
1	B	1484	ALA	3.9
1	C	1640	GLN	3.9
1	A	1650	ASP	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1653	PHE	3.9
1	C	1690	ILE	3.9
1	B	1730	CYS	3.8
1	C	1677	THR	3.8
1	C	1637	PRO	3.8
1	B	1677	THR	3.8
1	C	1664	GLU	3.8
1	B	1681	VAL	3.8
1	A	2048	ASP	3.8
1	B	1486	PRO	3.7
1	C	2042	ASP	3.7
1	A	1686	GLU	3.7
1	B	2033	ILE	3.7
1	B	2084	PRO	3.7
1	A	2083	LEU	3.7
1	A	2086	TYR	3.7
1	C	1678	GLU	3.7
1	B	2044	MET	3.7
1	A	1644	ASN	3.7
1	C	1659	THR	3.7
1	C	1639	PHE	3.6
1	C	2086	TYR	3.6
1	B	1485	THR	3.6
1	B	1640	GLN	3.6
1	A	1679	ARG	3.6
1	C	1644	ASN	3.6
1	C	1836	THR	3.6
1	C	1688	PHE	3.6
1	C	2040	LEU	3.6
1	C	2047	LEU	3.6
1	A	1687	ARG	3.5
1	C	2035	PHE	3.5
1	B	1663	MET	3.5
1	C	1498	TYR	3.5
1	C	2184	ASP	3.5
1	C	1651	LYS	3.5
1	A	1689	VAL	3.5
1	C	1495	PRO	3.5
1	B	1690	ILE	3.4
1	C	1649	PRO	3.4
1	A	1688	PHE	3.4
1	B	1676	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1667	LYS	3.4
1	C	2191	LEU	3.4
1	A	1484	ALA	3.4
1	C	1675	VAL	3.4
1	B	1910	PRO	3.4
1	A	2041	LEU	3.3
1	C	1672	GLU	3.3
1	A	1481	ARG	3.3
1	C	1646	ALA	3.3
1	C	1643	TRP	3.3
1	C	1653	PHE	3.2
1	B	2134	TYR	3.2
1	B	2042	ASP	3.2
1	B	1913	ALA	3.2
1	C	2044	MET	3.2
1	B	1679	ARG	3.2
1	C	2046	ARG	3.2
1	A	1639	PHE	3.2
1	C	1665	THR	3.2
1	B	2145	GLU	3.2
1	B	1648	ASN	3.1
1	C	1691	LYS	3.1
1	B	2032	GLY	3.1
1	C	1769	GLU	3.1
1	C	2043	THR	3.1
1	B	2035	PHE	3.1
1	A	2191	LEU	3.1
1	B	1639	PHE	3.1
1	A	1648	ASN	3.1
1	A	1663	MET	3.1
1	C	2049	ASP	3.1
1	C	1689	VAL	3.0
1	A	1911	ASN	3.0
1	B	2040	LEU	3.0
1	C	2085	ILE	3.0
1	C	1633	GLU	3.0
1	C	1656	LEU	3.0
1	A	1669	PHE	3.0
1	B	1824	LYS	3.0
1	A	1656	LEU	3.0
1	C	1916	LEU	3.0
1	A	1690	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1683	ASN	2.9
1	C	1911	ASN	2.9
1	B	1656	LEU	2.9
1	C	2142	GLN	2.9
1	B	1675	VAL	2.9
1	C	1632	ALA	2.9
1	B	2088	GLN	2.9
1	C	1661	GLU	2.9
1	A	1642	ALA	2.9
1	B	1521	SER	2.9
1	C	1692	THR	2.9
1	C	1696	SER	2.9
1	A	1485	THR	2.9
1	B	1960	GLN	2.8
1	C	1501	HIS	2.8
1	A	1638	LEU	2.8
1	B	1658	LEU	2.8
1	B	1692	THR	2.8
1	C	1658	LEU	2.8
1	C	1494	GLN	2.8
1	B	1531	LYS	2.8
1	B	1678	GLU	2.8
1	B	1487	TYR	2.8
1	C	2149	LEU	2.8
1	B	1659	THR	2.8
1	C	2162	SER	2.8
1	C	1693	ILE	2.8
1	C	1533	THR	2.8
1	A	1691	LYS	2.8
1	B	2163	VAL	2.8
1	C	2141	HIS	2.7
1	C	1531	LYS	2.7
1	B	1525	ASN	2.7
1	A	2049	ASP	2.7
1	C	1852	THR	2.7
1	B	2157	SER	2.7
1	A	1645	ASP	2.7
1	B	1654	GLN	2.7
1	C	1854	SER	2.7
1	C	1635	ILE	2.7
1	A	1486	PRO	2.7
1	C	2189	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2161	ALA	2.6
1	C	1559	ALA	2.6
1	B	2097	HIS	2.6
1	B	1691	LYS	2.6
1	C	1502	LEU	2.6
1	C	1642	ALA	2.6
1	B	2037	ARG	2.6
1	A	1665	THR	2.6
1	B	2091	LEU	2.6
1	A	2044	MET	2.6
1	B	1669	PHE	2.6
1	A	1657	TYR	2.6
1	B	1767	GLY	2.6
1	A	2089	ILE	2.6
1	C	2192	GLU	2.6
1	A	1667	LYS	2.6
1	C	2187	LYS	2.6
1	A	2037	ARG	2.5
1	A	1652	GLY	2.5
1	B	1488	PRO	2.5
1	C	1657	TYR	2.5
1	C	1650	ASP	2.5
1	C	1668	LYS	2.5
1	C	1764	LYS	2.5
1	A	2084	PRO	2.5
1	A	1685	GLU	2.5
1	B	2141	HIS	2.5
1	C	1648	ASN	2.5
1	C	1671	LYS	2.5
1	B	1958	GLY	2.5
1	A	1960	GLN	2.5
1	A	1677	THR	2.5
1	B	2034	LYS	2.5
1	B	2098	ASP	2.4
1	B	2189	LEU	2.4
1	C	1631	MET	2.4
1	A	2085	ILE	2.4
1	B	2093	PHE	2.4
1	C	1669	PHE	2.4
1	A	1676	LEU	2.4
1	A	2091	LEU	2.4
1	A	2039	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1671	LYS	2.4
1	B	2160	PRO	2.4
1	A	1662	GLY	2.4
1	B	2031	VAL	2.4
1	B	1674	SER	2.4
1	A	1658	LEU	2.4
1	A	1668	LYS	2.4
1	C	1772	THR	2.4
1	B	1666	LEU	2.4
1	B	2188	GLY	2.3
1	B	1657	TYR	2.3
1	C	1766	LEU	2.3
1	C	2089	ILE	2.3
1	B	2027	PRO	2.3
1	A	2142	GLN	2.3
1	B	1912	SER	2.3
1	B	1685	GLU	2.3
1	A	1692	THR	2.3
1	B	1693	ILE	2.3
1	B	2089	ILE	2.3
1	B	1695	GLY	2.3
1	A	1913	ALA	2.2
1	B	2028	GLN	2.2
1	C	1838	ASP	2.2
1	B	1652	GLY	2.2
1	B	2146	ALA	2.2
1	B	2153	ALA	2.2
1	C	1667	LYS	2.2
1	A	1907	PRO	2.2
1	B	1770	VAL	2.2
1	B	2179	TYR	2.2
1	B	1662	GLY	2.2
1	A	2040	LEU	2.2
1	B	1857	GLU	2.2
1	C	2096	LEU	2.2
1	B	1673	ASN	2.2
1	B	1961	ARG	2.2
1	C	1960	GLN	2.2
1	B	2116	THR	2.2
1	A	2093	PHE	2.2
1	C	2185	LYS	2.2
1	A	1480	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1664	GLU	2.2
1	B	2036	ARG	2.2
1	C	1694	ILE	2.2
1	A	2141	HIS	2.2
1	B	1489	VAL	2.2
1	A	2035	PHE	2.2
1	B	1771	TYR	2.2
1	B	2094	ALA	2.2
1	A	1631	MET	2.1
1	C	2034	LYS	2.1
1	C	2190	LYS	2.1
1	A	1630	GLY	2.1
1	C	2188	GLY	2.1
1	B	2039	LYS	2.1
1	A	1767	GLY	2.1
1	A	2087	GLY	2.1
1	C	1556	GLU	2.1
1	C	1654	GLN	2.1
1	A	1961	ARG	2.1
1	B	1635	ILE	2.1
1	B	1911	ASN	2.1
1	C	2091	LEU	2.1
1	C	1942	GLY	2.1
1	A	2042	ASP	2.1
1	B	1836	THR	2.1
1	B	2164	ASP	2.1
1	B	2158	TRP	2.1
1	C	1634	GLU	2.1
1	C	1685	GLU	2.1
1	A	1487	TYR	2.1
1	A	2088	GLN	2.0
1	B	1765	MET	2.0
1	A	1675	VAL	2.0
1	B	1699	GLY	2.0
1	C	1915	THR	2.0
1	B	1632	ALA	2.0
1	C	1575	GLU	2.0
1	A	1916	LEU	2.0
1	C	1493	LEU	2.0
1	C	1902	LEU	2.0
1	A	1941	ASN	2.0
1	A	2046	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2033	ILE	2.0
1	B	1668	LYS	2.0
1	C	1499	LYS	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](#)

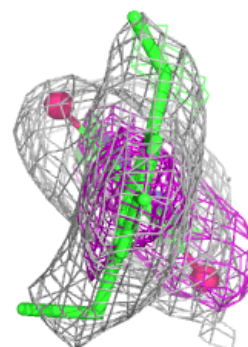
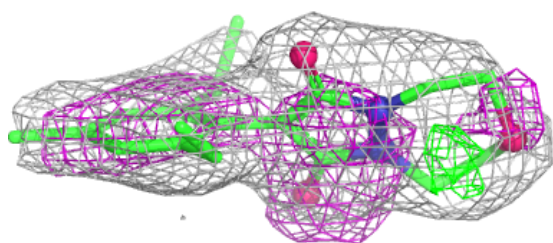
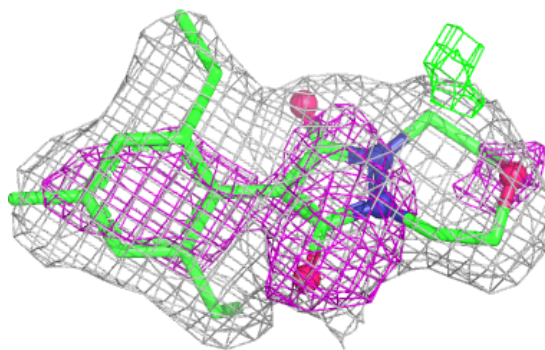
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GY3	A	3000	23/23	0.89	0.17	59,66,79,86	0
2	GY3	B	2240	23/23	0.89	0.23	139,156,186,191	0
2	GY3	B	3000	23/23	0.94	0.16	104,116,138,147	0

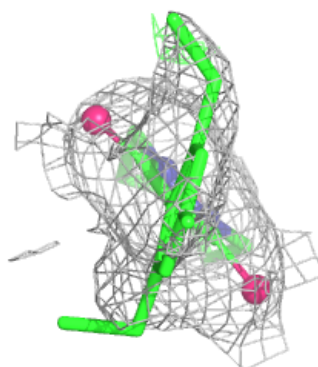
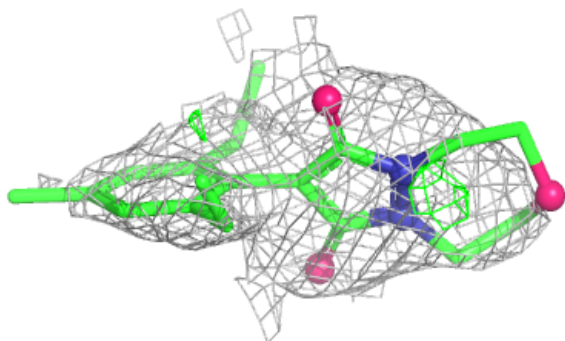
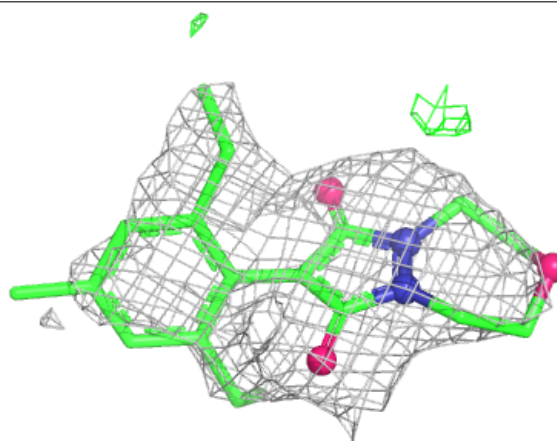
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GY3 A 3000:

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

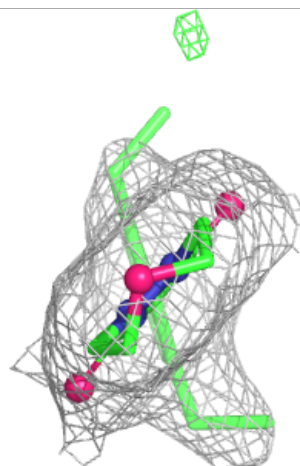
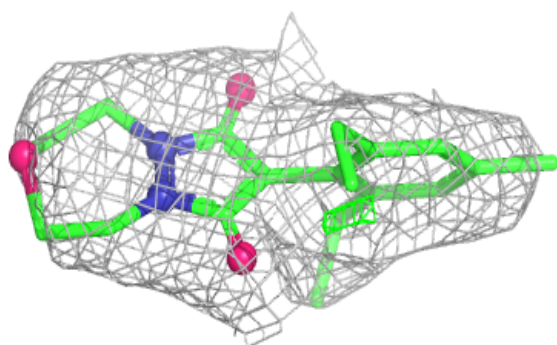
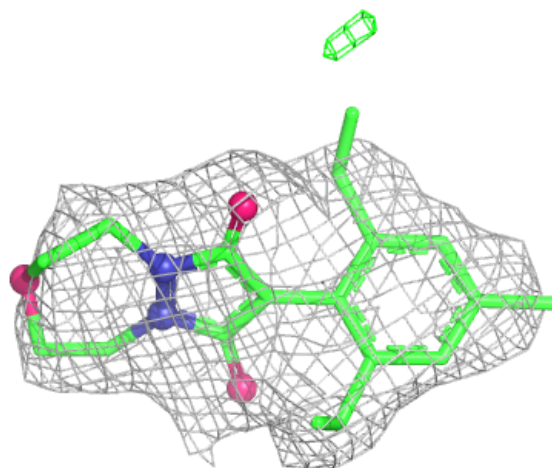
**Electron density around GY3 B 2240:**

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



Electron density around 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.