Full wwPDB X-ray Structure Validation Report (i)

Feb 12, 2024 – 05:08 AM EST

PDB ID	:	3H0Q
Title	:	Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 3
Authors	:	Zhang, H.; Tong, L.
Deposited on	:	2009-04-10
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

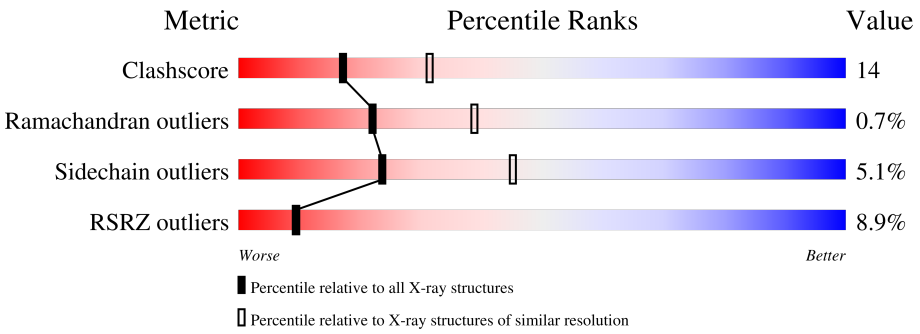
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	769	6% 65% 21% • 11%
1	B	769	9% 62% 23% • 12%
1	C	769	8% 62% 22% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16890 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
			Total	C	N	O	S			
1	A	681	5424	3459	930	1016	19	0	0	0
1	B	675	5376	3427	923	1007	19	0	0	0
1	C	665	5298	3374	912	993	19	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

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

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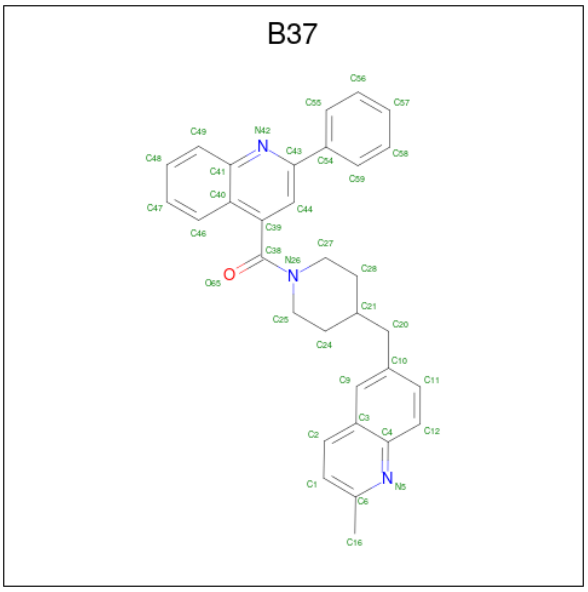
Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression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

- Molecule 2 is 4-({4-[(2-methylquinolin-6-yl)methyl]piperidin-1-yl}carbonyl)-2-phenylquinoline (three-letter code: B37) (formula: $C_{32}H_{29}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	36	32	3	1	0	0
			Total	C	N	O		
2	B	1	36	32	3	1	0	0
			Total	C	N	O		
2	C	1	36	32	3	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	252	252	252	0	0

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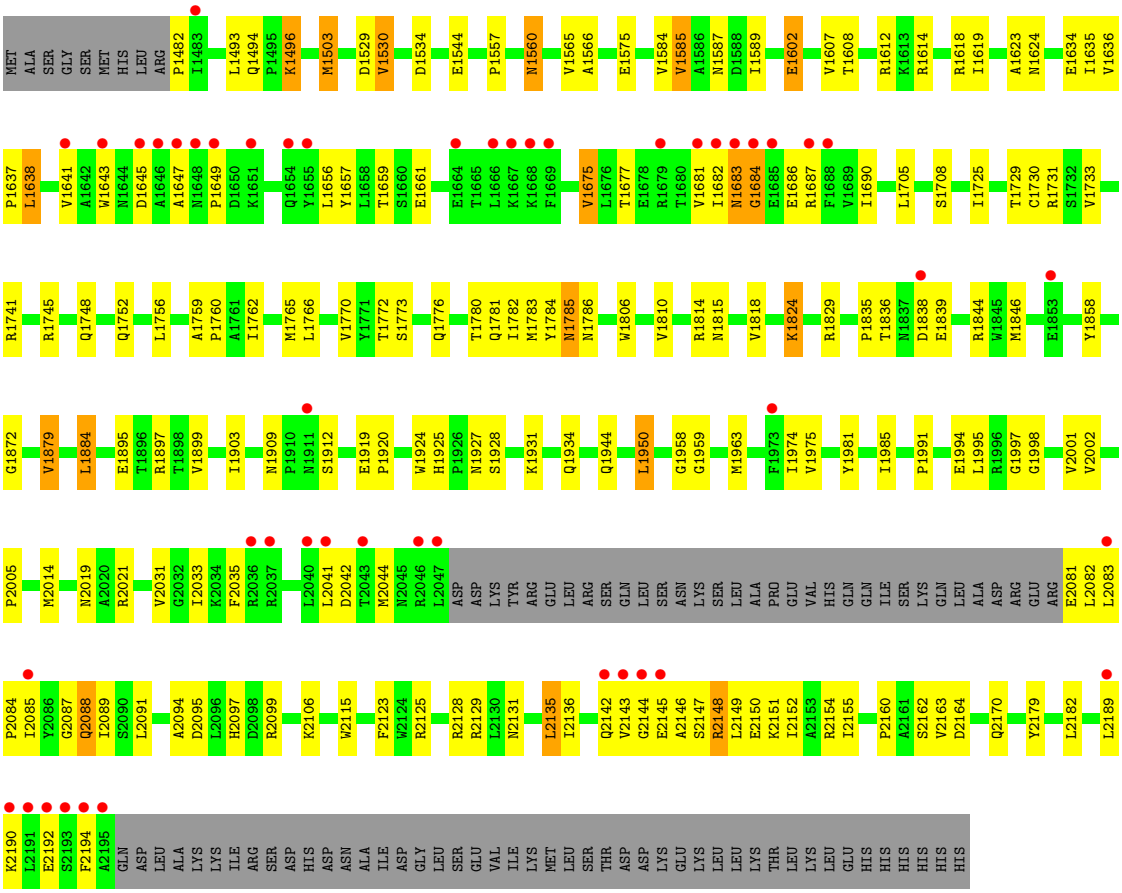
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	222	222	222	0	0
			Total	O		
3	C	210	210	210	0	0

3 Residue-property plots (i)

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.

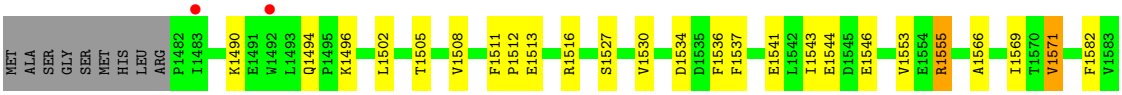
- Molecule 1: Acetyl-CoA carboxylase

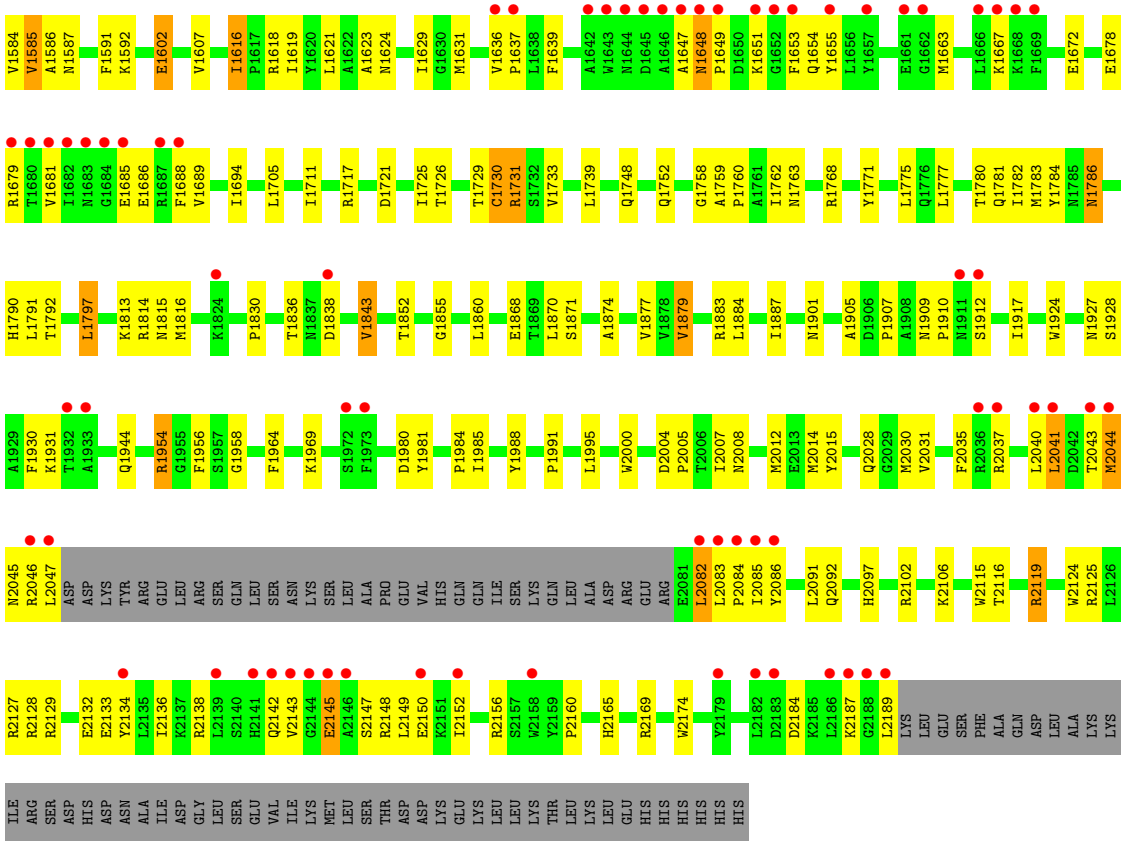
Chain A:



- Molecule 1: Acetyl-CoA carboxylase

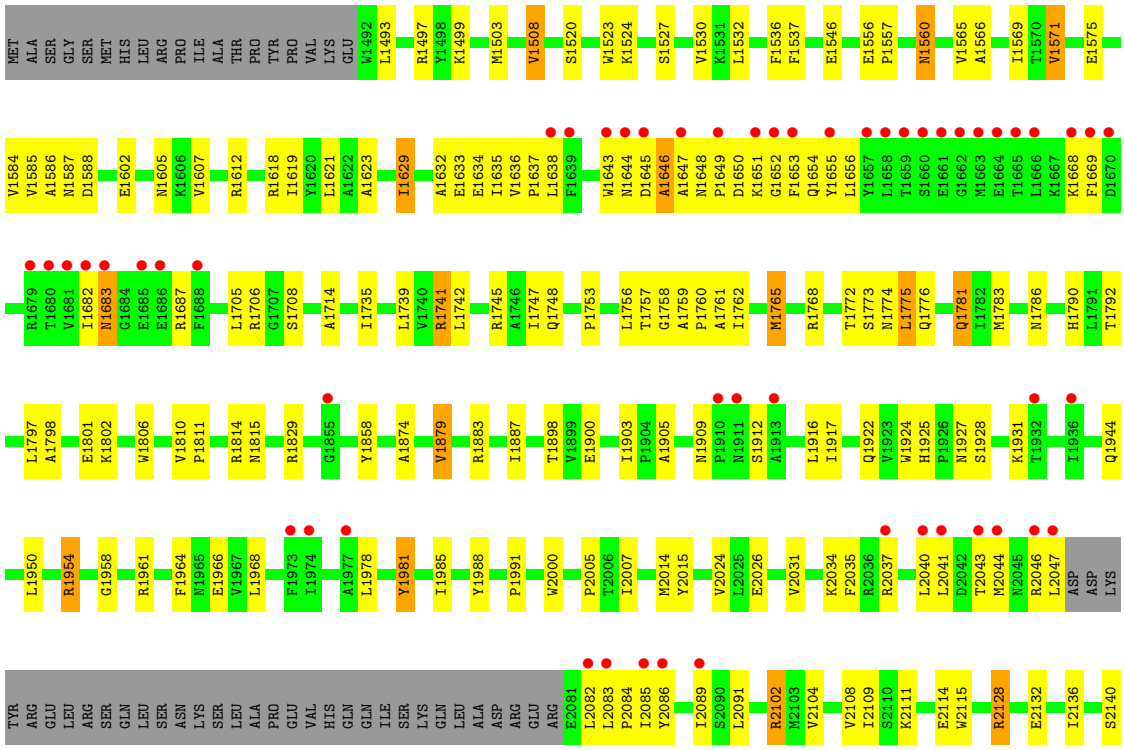
Chain B:

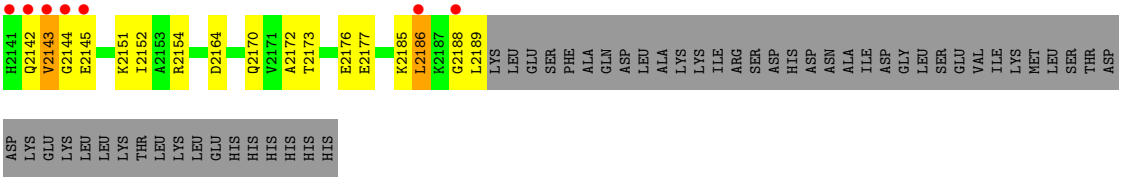




• Molecule 1: Acetyl-CoA carboxylase

Chain C: 8% 62% 22% • 14%




H2141
Q2142
V2143
G2144
E2145
K2151
I2152
A2153
R2154
D2164
Q2170
V2171
A2172
T2173
E2176
E2177
K2185
L2186
K2187
G2188
L2189
LYS
LEU
GLU
SER
PHE
ALA
GLN
ASP
LEU
ALA
LYS
LYS
ILE
ARG
SER
ASP
HIS
ASP
ASN
ALA
ILE
ASP
GLY
LEU
SER
GLU
VAL
ILE
LYS
MET
LEU
SER
THR
ASP
ASP
LYS
GLU
LYS
LEU
LEU
LYS
THR
LEU
LYS
LEU
GLU
HIS
HIS
HIS
HIS
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.95Å 124.25Å 145.27Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	48.72 – 2.50 48.72 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.72-2.50) 91.1 (48.72-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.84 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.233 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16890	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B37

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	0.33	0/5546	0.61	0/7514
1	B	0.32	0/5497	0.62	0/7449
1	C	0.31	0/5415	0.61	1/7335 (0.0%)
All	All	0.32	0/16458	0.61	1/22298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1968	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5424	0	5365	149	0
1	B	5376	0	5316	161	0
1	C	5298	0	5234	163	0
2	A	36	0	29	4	0
2	B	36	0	29	5	0
2	C	36	0	29	2	0
3	A	252	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	222	0	0	4	0
3	C	210	0	0	4	0
All	All	16890	0	16002	449	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (449) 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	1.16	1.05
1:A:1772:THR:H	1:A:1776:GLN:HE22	1.11	0.96
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.64	0.94
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.95	0.93
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.14	0.91
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.10	0.90
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.69	0.90
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	1.86	0.89
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.18	0.88
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.19	0.87
1:A:1975:VAL:HG23	1:A:2002:VAL:HG23	1.56	0.87
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.54	0.87
1:A:1637:PRO:HG2	1:A:1638:LEU:HD23	1.59	0.84
1:B:1667:LYS:HD3	1:B:1672:GLU:HB3	1.59	0.84
1:C:1560:ASN:HD22	1:C:1560:ASN:H	1.25	0.84
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.76	0.83
1:A:1560:ASN:H	1:A:1560:ASN:HD22	1.26	0.83
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.25	0.82
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.60	0.81
1:B:1585:VAL:HG13	1:B:1607:VAL:HG11	1.62	0.81
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.63	0.80
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.65	0.79
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.79	0.79
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.66	0.78
1:B:2184:ASP:HA	1:B:2187:LYS:HD3	1.65	0.76
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.50	0.76
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.67	0.74
1:B:1541:GLU:OE1	1:B:1555:ARG:HD3	1.88	0.74
1:A:1656:LEU:HB2	1:A:1690:ILE:HD11	1.71	0.73
1:B:1730:CYS:CA	1:B:1752:GLN:HE21	2.02	0.72
1:C:1682:ILE:HG21	1:C:1687:ARG:HH11	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1647:ALA:O	1:B:1648:ASN:HB2	1.90	0.72
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.39	0.71
1:A:2082:LEU:HD23	1:A:2082:LEU:H	1.56	0.71
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.37	0.70
1:A:2041:LEU:HA	1:A:2044:MET:HG2	1.72	0.70
1:A:1496:LYS:H	1:A:1496:LYS:HD3	1.56	0.70
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.38	0.70
1:B:1624:ASN:ND2	1:B:1733:VAL:H	1.90	0.69
1:C:1646:ALA:C	1:C:1648:ASN:H	1.96	0.69
1:C:2005:PRO:HG3	1:C:2014:MET:HB2	1.72	0.69
1:C:1527:SER:O	1:C:1530:VAL:HG22	1.92	0.69
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.40	0.69
1:A:1991:PRO:O	1:A:2019:ASN:O	2.11	0.69
1:B:2008:ASN:H	1:B:2012:MET:HE3	1.58	0.68
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.23	0.68
1:A:1645:ASP:OD2	1:A:1647:ALA:HB3	1.94	0.68
1:A:2154:ARG:HH11	1:A:2189:LEU:HD21	1.58	0.68
1:B:2085:ILE:HG13	1:C:1650:ASP:HA	1.75	0.67
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.41	0.67
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.91	0.67
1:B:2152:ILE:O	1:B:2156:ARG:HG2	1.94	0.67
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.78	0.66
1:B:2008:ASN:N	1:B:2012:MET:HE3	2.10	0.66
1:B:2007:ILE:HB	1:B:2012:MET:HE1	1.78	0.66
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.31	0.65
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.27	0.65
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.93	0.65
1:A:1496:LYS:H	1:A:1496:LYS:CD	2.09	0.65
1:A:1958:GLY:H	2:A:1:B37:C2	2.09	0.65
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.77	0.65
1:B:1958:GLY:H	2:B:1:B37:C1	2.10	0.65
1:A:1560:ASN:H	1:A:1560:ASN:ND2	1.93	0.64
1:A:1975:VAL:CG2	1:A:2002:VAL:HG23	2.26	0.64
1:C:1745:ARG:HG2	1:C:1806:TRP:CZ2	2.33	0.64
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.12	0.64
1:A:1585:VAL:CG1	1:A:1607:VAL:HG11	2.29	0.63
1:C:1682:ILE:CG2	1:C:1687:ARG:HH11	2.12	0.63
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.97	0.63
1:A:1657:TYR:CZ	1:A:1687:ARG:HD2	2.34	0.63
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.43	0.62
1:B:1663:MET:O	1:B:1667:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.79	0.62
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.82	0.62
1:C:1773:SER:N	1:C:1776:GLN:HE21	1.96	0.62
1:C:1909:ASN:HD22	1:C:1912:SER:HB2	1.65	0.62
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.34	0.61
1:A:2162:SER:OG	1:B:1797:LEU:HB3	1.99	0.61
1:B:1730:CYS:H	1:B:1752:GLN:HG3	1.64	0.61
1:C:1797:LEU:O	1:C:1801:GLU:HG3	2.00	0.61
1:B:1513:GLU:OE1	1:B:1516:ARG:NH1	2.33	0.61
1:C:2164:ASP:H	1:C:2170:GLN:NE2	1.97	0.61
1:A:1683:ASN:CG	1:A:1684:GLY:H	2.04	0.61
1:C:2188:GLY:C	1:C:2189:LEU:HD12	2.21	0.61
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	1.82	0.61
1:A:1675:VAL:HG13	1:A:1677:THR:HG23	1.83	0.60
1:C:2142:GLN:HE22	1:C:2189:LEU:HB2	1.67	0.60
1:B:1877:VAL:HG13	1:B:1931:LYS:HD3	1.82	0.60
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.31	0.59
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.85	0.59
1:C:2005:PRO:CG	1:C:2014:MET:HB2	2.31	0.59
1:C:1644:ASN:HB2	1:C:1654:GLN:HG3	1.85	0.59
1:A:1494:GLN:HE22	1:A:1557:PRO:HD2	1.68	0.59
1:A:1494:GLN:HB3	1:A:1496:LYS:NZ	2.18	0.58
1:C:1745:ARG:NH2	3:C:2:HOH:O	2.24	0.58
1:C:1560:ASN:H	1:C:1560:ASN:ND2	1.96	0.58
1:A:2087:GLY:O	1:A:2091:LEU:HD13	2.03	0.58
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.04	0.58
1:A:2148:ARG:HG3	1:A:2149:LEU:N	2.17	0.58
1:B:1679:ARG:NH2	1:B:1686:GLU:HG3	2.18	0.58
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.85	0.58
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.06	0.57
1:A:1637:PRO:HG2	1:A:1638:LEU:CD2	2.30	0.57
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.03	0.57
1:B:2184:ASP:HA	1:B:2187:LYS:CD	2.34	0.57
1:A:1494:GLN:HB3	1:A:1496:LYS:CE	2.35	0.57
1:C:1644:ASN:HB2	1:C:1654:GLN:CG	2.33	0.57
1:B:1678:GLU:O	1:B:1689:VAL:HG12	2.04	0.57
1:A:1997:GLY:O	1:A:2001:VAL:HG23	2.05	0.56
1:B:1717:ARG:NH2	1:C:2007:ILE:O	2.30	0.56
1:B:2041:LEU:HD13	1:B:2044:MET:HE3	1.87	0.56
1:B:2044:MET:SD	1:B:2082:LEU:HD11	2.45	0.56
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:VAL:HG22	3:A:394:HOH:O	2.04	0.56
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.02	0.56
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.05	0.56
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.36	0.56
1:A:2142:GLN:HE22	1:A:2190:LYS:CG	2.19	0.56
1:C:1636:VAL:HB	1:C:1637:PRO:HD3	1.87	0.56
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.87	0.55
1:C:1790:HIS:HD2	3:C:64:HOH:O	1.89	0.55
1:C:1925:HIS:HD2	3:C:151:HOH:O	1.89	0.55
1:C:2037:ARG:HH21	1:C:2041:LEU:HD11	1.70	0.55
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.72	0.55
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.06	0.55
1:C:1587:ASN:ND2	1:C:1623:ALA:H	2.04	0.55
1:B:2083:LEU:HB2	1:B:2084:PRO:HD3	1.89	0.55
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.10	0.55
1:B:2044:MET:HA	1:B:2086:TYR:CE2	2.42	0.55
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.36	0.55
1:C:1556:GLU:HG3	1:C:1557:PRO:HD2	1.88	0.55
1:C:1905:ALA:HB1	1:C:1912:SER:OG	2.07	0.55
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.89	0.55
1:A:2031:VAL:HG11	1:A:2091:LEU:HD12	1.88	0.54
1:B:1585:VAL:CG1	1:B:1607:VAL:HG11	2.35	0.54
1:B:2046:ARG:HH22	1:C:1637:PRO:C	2.10	0.54
1:B:2040:LEU:HD11	1:B:2086:TYR:HB3	1.90	0.54
1:C:1647:ALA:O	1:C:1649:PRO:HD3	2.08	0.54
1:C:2185:LYS:O	1:C:2189:LEU:HD13	2.08	0.54
1:C:1637:PRO:HG2	1:C:1638:LEU:CD1	2.37	0.54
1:C:1643:TRP:CD1	1:C:1649:PRO:HA	2.43	0.54
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.90	0.54
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.73	0.54
1:B:1730:CYS:N	1:B:1752:GLN:HE21	2.05	0.54
1:B:1958:GLY:H	2:B:1:B37:C2	2.21	0.53
1:A:1494:GLN:HB3	1:A:1496:LYS:HE2	1.91	0.53
1:A:1657:TYR:CD2	1:A:1687:ARG:HB3	2.43	0.53
1:B:1730:CYS:H	1:B:1752:GLN:CG	2.20	0.53
1:C:1637:PRO:HG2	1:C:1638:LEU:HD12	1.89	0.53
1:C:1759:ALA:N	1:C:1774:ASN:HD21	1.93	0.53
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	1.89	0.53
1:C:1798:ALA:O	1:C:1802:LYS:HG2	2.08	0.53
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.05	0.53
1:C:1757:THR:HB	1:C:1762:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.09	0.53
1:A:1958:GLY:H	2:A:1:B37:C1	2.22	0.53
1:B:1782:ILE:O	1:B:1786:ASN:HB2	2.09	0.53
1:B:2037:ARG:HA	1:B:2040:LEU:HB3	1.91	0.53
1:A:1602:GLU:HG3	3:A:346:HOH:O	2.08	0.53
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.91	0.52
1:A:1682:ILE:O	1:A:1684:GLY:N	2.43	0.52
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	1.90	0.52
1:C:1643:TRP:HA	1:C:1653:PHE:HA	1.90	0.52
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.38	0.52
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.10	0.52
1:A:2142:GLN:HE22	1:A:2190:LYS:HG2	1.74	0.52
1:A:1838:ASP:O	1:A:1839:GLU:HG3	2.10	0.52
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.91	0.52
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.24	0.52
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.13	0.52
1:A:2095:ASP:O	1:A:2099:ARG:HD3	2.09	0.52
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.90	0.52
1:B:2143:VAL:HG23	1:B:2143:VAL:O	2.10	0.52
1:B:1729:THR:O	1:B:1730:CYS:HB3	2.10	0.52
1:C:1560:ASN:HD22	1:C:1560:ASN:N	2.03	0.52
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.91	0.51
1:A:1909:ASN:HD22	1:A:1912:SER:HB3	1.75	0.51
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.10	0.51
1:B:2082:LEU:HD13	1:B:2086:TYR:CD1	2.45	0.51
1:C:1493:LEU:HB2	1:C:1497:ARG:NH1	2.26	0.51
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.56	0.51
1:B:2041:LEU:HA	1:B:2044:MET:HE3	1.91	0.51
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.45	0.51
1:A:2192:GLU:HG2	1:A:2192:GLU:O	2.10	0.51
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.10	0.51
1:A:1496:LYS:HD3	1:A:1496:LYS:N	2.25	0.51
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.08	0.51
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.46	0.51
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.93	0.51
1:B:1667:LYS:CD	1:B:1672:GLU:HB3	2.38	0.51
1:B:1830:PRO:HB3	1:B:2116:THR:HG23	1.92	0.51
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.14	0.50
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.31	0.50
1:C:2040:LEU:O	1:C:2043:THR:HG22	2.10	0.50
1:A:2088:GLN:HE21	1:A:2088:GLN:CA	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	1.94	0.50
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	1.91	0.50
1:C:1645:ASP:O	1:C:1646:ALA:HB2	2.11	0.50
1:B:2031:VAL:HG21	1:B:2091:LEU:HD12	1.93	0.50
1:C:1508:VAL:HG11	1:C:1565:VAL:CG2	2.42	0.50
1:C:1768:ARG:HG2	1:C:1768:ARG:HH11	1.77	0.50
1:A:1682:ILE:HG12	1:A:1683:ASN:OD1	2.12	0.50
1:A:1991:PRO:CG	1:A:2115:TRP:HB2	2.38	0.50
1:B:1860:LEU:O	1:B:2119:ARG:HG2	2.12	0.50
1:C:2041:LEU:HA	1:C:2044:MET:CG	2.42	0.50
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.29	0.50
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.93	0.50
1:A:1903:ILE:N	1:A:1903:ILE:HD12	2.26	0.50
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.74	0.50
1:A:2095:ASP:OD2	1:A:2099:ARG:NH1	2.45	0.50
1:A:2143:VAL:HG23	1:A:2192:GLU:OE1	2.11	0.50
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.47	0.50
1:C:1958:GLY:H	2:C:1:B37:C2	2.25	0.50
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.43	0.49
1:B:1758:GLY:O	1:B:1762:ILE:HG12	2.12	0.49
1:A:1785:ASN:HD22	1:A:1785:ASN:N	2.10	0.49
1:B:1786:ASN:ND2	1:C:1964:PHE:O	2.41	0.49
1:A:2106:LYS:HA	1:A:2106:LYS:HE2	1.93	0.49
1:C:2047:LEU:C	1:C:2047:LEU:HD13	2.32	0.49
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.94	0.49
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.13	0.49
1:A:1974:ILE:HB	1:A:2002:VAL:HG21	1.93	0.49
1:B:1653:PHE:CZ	1:C:2089:ILE:HD13	2.48	0.49
1:B:1775:LEU:O	1:B:1781:GLN:NE2	2.42	0.49
1:B:1901:ASN:HB3	1:B:1917:ILE:HB	1.93	0.49
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.77	0.49
1:A:1681:VAL:HG12	1:A:1686:GLU:HA	1.95	0.49
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.11	0.49
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.61	0.49
1:A:1927:ASN:OD1	1:A:1928:SER:N	2.45	0.49
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.13	0.49
1:A:1656:LEU:O	1:A:1690:ILE:HG12	2.13	0.48
1:A:1909:ASN:ND2	1:A:1912:SER:HB3	2.28	0.48
1:B:2043:THR:C	1:B:2045:ASN:H	2.16	0.48
1:B:1786:ASN:ND2	1:C:1966:GLU:HG3	2.28	0.48
1:B:1843:VAL:HG22	3:B:10:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:HD23	1:A:1770:VAL:HG21	1.95	0.48
1:C:1922:GLN:O	1:C:1954:ARG:HG2	2.13	0.48
1:A:1682:ILE:HG21	1:A:1687:ARG:CZ	2.43	0.48
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.62	0.48
1:B:1711:ILE:HD12	1:B:1739:LEU:HD11	1.95	0.48
1:B:2046:ARG:NH2	1:C:1637:PRO:O	2.45	0.48
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.95	0.48
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.14	0.48
1:B:2030:MET:HE3	1:B:2030:MET:HA	1.95	0.48
1:C:2031:VAL:HG21	1:C:2091:LEU:HD23	1.95	0.48
1:A:1682:ILE:O	1:A:1683:ASN:C	2.51	0.47
1:A:1766:LEU:N	1:A:1766:LEU:HD12	2.29	0.47
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.14	0.47
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.44	0.47
1:C:2143:VAL:HG23	1:C:2143:VAL:O	2.13	0.47
1:C:1668:LYS:HE3	1:C:1669:PHE:CE2	2.49	0.47
1:A:1634:GLU:O	1:A:1638:LEU:HD21	2.14	0.47
1:B:2124:TRP:CE3	1:B:2169:ARG:HA	2.49	0.47
1:C:1632:ALA:HB1	1:C:1634:GLU:OE2	2.14	0.47
1:C:1633:GLU:HA	1:C:1636:VAL:HG23	1.97	0.47
1:C:2142:GLN:NE2	1:C:2189:LEU:HB2	2.30	0.47
1:B:1624:ASN:HD21	1:B:1733:VAL:N	2.09	0.47
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.44	0.47
1:A:2147:SER:OG	1:A:2150:GLU:HG3	2.15	0.47
1:C:2142:GLN:O	1:C:2144:GLY:N	2.48	0.47
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.45	0.47
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.96	0.47
1:A:2033:ILE:HD11	2:A:1:B37:H58	1.95	0.47
1:A:2041:LEU:HA	1:A:2044:MET:CG	2.44	0.47
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.97	0.47
3:B:683:HOH:O	1:C:1765:MET:HE2	2.14	0.47
1:C:1635:ILE:HG22	1:C:1635:ILE:O	2.14	0.47
1:B:1544:GLU:OE2	1:B:1602:GLU:OE1	2.33	0.46
1:C:1520:SER:O	1:C:1524:LYS:HG2	2.14	0.46
1:C:1768:ARG:HG2	1:C:1768:ARG:NH1	2.30	0.46
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.97	0.46
1:C:2041:LEU:HA	1:C:2044:MET:HG2	1.97	0.46
1:C:2172:ALA:O	1:C:2176:GLU:HG3	2.16	0.46
1:B:1909:ASN:HD22	1:B:1912:SER:HB2	1.80	0.46
1:B:2041:LEU:HD22	1:B:2044:MET:CE	2.45	0.46
1:B:2143:VAL:HB	1:B:2145:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1730:CYS:O	1:B:1731:ARG:O	2.33	0.46
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.97	0.46
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.31	0.46
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.16	0.46
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.98	0.46
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.19	0.46
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.45	0.46
1:A:1529:ASP:O	1:A:1530:VAL:C	2.53	0.46
1:A:1560:ASN:ND2	1:A:1560:ASN:N	2.62	0.46
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.31	0.46
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.51	0.46
1:A:2146:ALA:O	1:A:2151:LYS:HE3	2.16	0.45
1:B:1852:THR:HG22	1:B:1855:GLY:O	2.16	0.45
1:B:2134:TYR:CZ	1:B:2138:ARG:HD2	2.51	0.45
1:B:2147:SER:HB3	1:B:2150:GLU:HG3	1.99	0.45
1:A:1683:ASN:CG	1:A:1684:GLY:N	2.69	0.45
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.81	0.45
1:C:1560:ASN:ND2	1:C:1560:ASN:N	2.61	0.45
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.16	0.45
1:B:1654:GLN:O	1:B:1655:TYR:HB3	2.16	0.45
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.97	0.45
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.46	0.45
1:C:2111:LYS:HB2	1:C:2111:LYS:HE3	1.77	0.45
1:C:1633:GLU:OE2	1:C:1636:VAL:HG21	2.16	0.45
1:B:1879:VAL:HG13	1:B:1931:LYS:HE2	1.99	0.45
1:B:1984:PRO:HD3	1:B:2133:GLU:HG3	1.98	0.45
1:B:2005:PRO:HG3	1:B:2014:MET:HB2	1.99	0.45
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.16	0.45
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.81	0.45
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.98	0.45
1:C:1629:ILE:HD13	1:C:1629:ILE:H	1.81	0.45
1:C:2085:ILE:HG23	1:C:2086:TYR:HD1	1.81	0.45
1:A:1503:MET:CE	1:A:1589:ILE:HG13	2.46	0.45
1:B:2134:TYR:CE1	1:B:2138:ARG:HD2	2.51	0.45
1:B:1909:ASN:ND2	1:B:1912:SER:N	2.65	0.45
1:C:1646:ALA:C	1:C:1648:ASN:N	2.64	0.45
1:A:1496:LYS:CD	1:A:1496:LYS:N	2.79	0.45
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	1.99	0.45
1:A:1705:LEU:O	1:A:1708:SER:HB3	2.16	0.45
1:C:1523:TRP:HB3	1:C:1530:VAL:HG21	1.97	0.45
1:B:1679:ARG:HH21	1:B:1686:GLU:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.80	0.44
1:A:2083:LEU:HB2	1:A:2084:PRO:HD3	1.99	0.44
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.18	0.44
1:C:1903:ILE:HG12	1:C:1917:ILE:HD13	1.98	0.44
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.52	0.44
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.52	0.44
1:C:2140:SER:OG	1:C:2151:LYS:HE2	2.17	0.44
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.18	0.44
1:B:1639:PHE:O	1:C:2046:ARG:NH1	2.51	0.44
1:C:1682:ILE:O	1:C:1683:ASN:C	2.55	0.44
1:C:1981:TYR:CG	1:C:1985:ILE:HD11	2.52	0.44
1:B:1679:ARG:O	1:B:1679:ARG:HG3	2.17	0.44
1:B:1768:ARG:HG2	1:B:1768:ARG:HH11	1.83	0.44
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.17	0.44
1:A:1730:CYS:O	1:A:1731:ARG:C	2.56	0.44
1:C:1682:ILE:HG21	1:C:1687:ARG:NH1	2.27	0.44
1:C:2083:LEU:N	1:C:2084:PRO:CD	2.81	0.44
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.53	0.43
1:C:1988:TYR:HA	1:C:2015:TYR:O	2.18	0.43
1:B:2045:ASN:O	1:B:2046:ARG:HD2	2.18	0.43
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.66	0.43
1:B:1647:ALA:O	1:B:1648:ASN:CB	2.63	0.43
1:C:1810:VAL:HG13	1:C:1811:PRO:HD2	1.99	0.43
1:B:1958:GLY:H	2:B:1:B37:H1	1.82	0.43
1:B:2028:GLN:H	1:B:2028:GLN:CD	2.22	0.43
1:A:1493:LEU:C	1:A:1494:GLN:HG3	2.38	0.43
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.34	0.43
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.84	0.43
1:A:1998:GLY:HA3	3:A:3:HOH:O	2.18	0.43
1:A:2082:LEU:O	1:A:2085:ILE:HG22	2.19	0.43
1:B:1653:PHE:CD1	1:B:1653:PHE:N	2.86	0.43
1:B:2132:GLU:O	1:B:2136:ILE:HG13	2.19	0.43
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.17	0.43
1:A:1824:LYS:HB2	1:A:1824:LYS:HE2	1.85	0.43
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.00	0.43
1:B:1681:VAL:HA	1:B:1685:GLU:O	2.18	0.43
1:B:1813:LYS:HG2	1:B:1816:MET:SD	2.59	0.43
1:B:1964:PHE:O	1:C:1786:ASN:OD1	2.36	0.43
1:A:2082:LEU:HD23	1:A:2082:LEU:N	2.30	0.43
1:A:1482:PRO:N	3:A:88:HOH:O	2.52	0.43
1:C:1753:PRO:HB3	1:C:1775:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2083:LEU:HB2	1:C:2084:PRO:HD3	2.01	0.43
1:A:1836:THR:HB	1:A:1839:GLU:HB2	2.00	0.43
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.18	0.43
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	2.00	0.42
1:C:1645:ASP:OD2	1:C:1652:GLY:O	2.37	0.42
1:C:1650:ASP:OD2	1:C:1651:LYS:HE3	2.18	0.42
1:C:2173:THR:O	1:C:2177:GLU:HG3	2.18	0.42
1:C:2186:LEU:HD12	1:C:2186:LEU:HA	1.80	0.42
1:B:2004:ASP:OD1	1:C:1706:ARG:HA	2.20	0.42
1:C:1874:ALA:HB2	1:C:1927:ASN:HB2	2.01	0.42
1:A:1494:GLN:CB	1:A:1496:LYS:NZ	2.83	0.42
1:A:2088:GLN:CA	1:A:2088:GLN:NE2	2.82	0.42
1:C:2085:ILE:O	1:C:2089:ILE:HG12	2.20	0.42
1:B:1530:VAL:O	1:B:1530:VAL:HG13	2.19	0.42
1:C:1499:LYS:O	1:C:1503:MET:HG2	2.19	0.42
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.50	0.42
1:B:1988:TYR:HA	1:B:2015:TYR:O	2.19	0.42
1:B:2156:ARG:HG3	1:B:2156:ARG:NH1	2.34	0.42
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.83	0.42
1:C:1758:GLY:O	1:C:1762:ILE:HG12	2.19	0.42
1:A:1920:PRO:HD2	1:A:1925:HIS:CE1	2.54	0.42
1:B:1586:ALA:CB	1:B:1621:LEU:HB2	2.49	0.42
1:B:1649:PRO:C	1:B:1651:LYS:H	2.23	0.42
2:B:1:B37:C55	1:C:1761:ALA:HA	2.50	0.42
1:C:2083:LEU:N	1:C:2083:LEU:HD12	2.35	0.42
1:A:1835:PRO:HG3	1:A:1846:MET:SD	2.59	0.42
1:C:2082:LEU:HD23	1:C:2082:LEU:HA	1.83	0.42
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.18	0.42
1:A:2094:ALA:HA	1:A:2097:HIS:HD2	1.85	0.42
1:B:1490:LYS:NZ	3:B:122:HOH:O	2.53	0.42
1:C:1927:ASN:OD1	1:C:1928:SER:N	2.51	0.42
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	2.01	0.42
1:B:1909:ASN:HA	1:B:1910:PRO:HD3	1.88	0.42
1:C:2026:GLU:OE2	2:C:1:B37:H46	2.20	0.42
1:C:2104:VAL:HG23	1:C:2109:ILE:HD11	2.01	0.42
1:A:1782:ILE:O	1:A:1786:ASN:HB2	2.20	0.42
1:C:1508:VAL:HG11	1:C:1565:VAL:HG22	2.02	0.42
1:C:1735:ILE:O	1:C:1739:LEU:HG	2.19	0.42
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.20	0.41
1:A:1958:GLY:H	2:A:1:B37:H2	1.82	0.41
1:A:2189:LEU:HD12	1:A:2189:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1527:SER:O	1:B:1530:VAL:HG12	2.20	0.41
1:C:1575:GLU:HG2	3:C:56:HOH:O	2.20	0.41
1:C:2189:LEU:HD12	1:C:2189:LEU:N	2.34	0.41
1:A:2162:SER:HG	1:B:1797:LEU:HB3	1.84	0.41
1:B:1786:ASN:HD22	1:B:1786:ASN:HA	1.54	0.41
1:B:2037:ARG:NH1	1:B:2041:LEU:HD21	2.35	0.41
1:B:2047:LEU:HD13	1:B:2047:LEU:C	2.41	0.41
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.53	0.41
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.35	0.41
1:C:1810:VAL:HA	1:C:1811:PRO:HD3	1.96	0.41
1:C:1917:ILE:HD12	1:C:1917:ILE:N	2.36	0.41
1:A:1638:LEU:HD23	1:A:1638:LEU:N	2.36	0.41
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.52	0.41
1:B:1729:THR:O	1:B:1729:THR:HG23	2.21	0.41
1:C:1634:GLU:O	1:C:1638:LEU:HD13	2.21	0.41
1:C:1705:LEU:O	1:C:1708:SER:HB2	2.20	0.41
1:B:1511:PHE:N	1:B:1512:PRO:CD	2.84	0.41
1:C:1747:ILE:HD13	1:C:1802:LYS:CB	2.49	0.41
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.84	0.41
1:B:1954:ARG:NH1	2:B:1:B37:H11	2.36	0.41
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.85	0.41
1:B:1591:PHE:O	1:B:1592:LYS:C	2.57	0.41
1:B:1663:MET:HG3	1:B:1688:PHE:CD2	2.55	0.41
1:B:1995:LEU:HD12	1:B:1995:LEU:HA	1.92	0.41
1:B:2000:TRP:CG	1:C:1705:LEU:HB3	2.56	0.41
1:C:2041:LEU:O	1:C:2044:MET:HB2	2.20	0.41
1:B:1705:LEU:HB3	1:C:2000:TRP:CG	2.56	0.41
1:B:2149:LEU:HD13	1:B:2149:LEU:C	2.41	0.41
1:C:1605:ASN:ND2	1:C:1714:ALA:HB2	2.36	0.41
1:C:1774:ASN:HD22	1:C:1774:ASN:HA	1.67	0.41
1:C:2154:ARG:HG3	1:C:2154:ARG:NH1	2.35	0.41
1:A:1614:ARG:HG3	1:A:1614:ARG:NH1	2.36	0.40
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	2.03	0.40
1:B:1629:ILE:HG22	1:C:2024:VAL:HB	2.03	0.40
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.51	0.40
1:A:1835:PRO:CG	1:A:1846:MET:SD	3.09	0.40
1:B:2125:ARG:O	1:B:2129:ARG:HG2	2.20	0.40
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.20	0.40
1:A:1659:THR:OG1	1:A:1661:GLU:HB3	2.22	0.40
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.21	0.40
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2119:ARG:HB3	3:B:77:HOH:O	2.21	0.40
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	2.03	0.40
1:C:1954:ARG:HG2	1:C:1954:ARG:H	1.71	0.40
1:A:1503:MET:HE2	1:A:1589:ILE:HG13	2.03	0.40
1:A:1950:LEU:HD12	1:A:1950:LEU:HA	1.96	0.40
1:B:2082:LEU:C	1:B:2082:LEU:HD12	2.41	0.40
1:B:2160:PRO:HD3	1:B:2174:TRP:CZ2	2.57	0.40
1:A:2170:GLN:OE1	1:B:1797:LEU:HD11	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	677/769 (88%)	636 (94%)	35 (5%)	6 (1%)	17	31
1	B	671/769 (87%)	627 (93%)	39 (6%)	5 (1%)	22	39
1	C	661/769 (86%)	622 (94%)	35 (5%)	4 (1%)	25	43
All	All	2009/2307 (87%)	1885 (94%)	109 (5%)	15 (1%)	22	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1530	VAL
1	A	1683	ASN
1	B	1731	ARG
1	C	2143	VAL
1	A	1684	GLY
1	A	2145	GLU
1	A	2194	PHE
1	B	2142	GLN
1	C	1646	ALA

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Mol	Chain	Res	Type
1	B	1730	CYS
1	C	2145	GLU
1	B	2044	MET
1	C	1683	ASN
1	B	1648	ASN
1	A	2144	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/658 (88%)	549 (95%)	28 (5%)	25	47
1	B	572/658 (87%)	539 (94%)	33 (6%)	20	38
1	C	563/658 (86%)	536 (95%)	27 (5%)	25	48
All	All	1712/1974 (87%)	1624 (95%)	88 (5%)	24	45

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1496	LYS
1	A	1503	MET
1	A	1534	ASP
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1618	ARG
1	A	1638	LEU
1	A	1641	VAL
1	A	1675	VAL
1	A	1756	LEU
1	A	1765	MET
1	A	1781	GLN
1	A	1785	ASN
1	A	1810	VAL
1	A	1824	LYS

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Mol	Chain	Res	Type
1	A	1879	VAL
1	A	1884	LEU
1	A	1924	TRP
1	A	1950	LEU
1	A	1995	LEU
1	A	2035	PHE
1	A	2042	ASP
1	A	2081	GLU
1	A	2088	GLN
1	A	2128	ARG
1	A	2135	LEU
1	A	2148	ARG
1	B	1502	LEU
1	B	1508	VAL
1	B	1534	ASP
1	B	1536	PHE
1	B	1555	ARG
1	B	1571	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1616	ILE
1	B	1618	ARG
1	B	1726	THR
1	B	1777	LEU
1	B	1786	ASN
1	B	1791	LEU
1	B	1792	THR
1	B	1797	LEU
1	B	1843	VAL
1	B	1879	VAL
1	B	1884	LEU
1	B	1924	TRP
1	B	1930	PHE
1	B	1954	ARG
1	B	1980	ASP
1	B	2035	PHE
1	B	2041	LEU
1	B	2082	LEU
1	B	2092	GLN
1	B	2119	ARG
1	B	2127	ARG
1	B	2128	ARG

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Mol	Chain	Res	Type
1	B	2145	GLU
1	B	2165	HIS
1	B	2189	LEU
1	C	1508	VAL
1	C	1532	LEU
1	C	1536	PHE
1	C	1560	ASN
1	C	1571	VAL
1	C	1602	GLU
1	C	1618	ARG
1	C	1629	ILE
1	C	1741	ARG
1	C	1742	LEU
1	C	1765	MET
1	C	1775	LEU
1	C	1781	GLN
1	C	1792	THR
1	C	1879	VAL
1	C	1898	THR
1	C	1924	TRP
1	C	1950	LEU
1	C	1954	ARG
1	C	1961	ARG
1	C	1978	LEU
1	C	1981	TYR
1	C	2035	PHE
1	C	2102	ARG
1	C	2114	GLU
1	C	2128	ARG
1	C	2186	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1624	ASN
1	A	1640	GLN
1	A	1644	ASN
1	A	1744	GLN

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Mol	Chain	Res	Type
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1785	ASN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1918	GLN
1	A	1934	GLN
1	A	2088	GLN
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	1599	GLN
1	B	1605	ASN
1	B	1624	ASN
1	B	1683	ASN
1	B	1744	GLN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1911	ASN
1	B	1934	GLN
1	B	1941	ASN
1	B	1944	GLN
1	B	2045	ASN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1587	ASN

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Mol	Chain	Res	Type
1	C	1605	ASN
1	C	1640	GLN
1	C	1654	GLN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1790	HIS
1	C	1815	ASN
1	C	1909	ASN
1	C	1911	ASN
1	C	1918	GLN
1	C	1941	ASN
1	C	1960	GLN
1	C	2011	GLN
1	C	2092	GLN
1	C	2142	GLN
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 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	B37	C	1	-	40,41,41	2.64	22 (55%)	52,58,58	1.64	7 (13%)
2	B37	B	1	-	40,41,41	2.65	23 (57%)	52,58,58	1.59	6 (11%)
2	B37	A	1	-	40,41,41	2.63	23 (57%)	52,58,58	1.69	8 (15%)

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	B37	C	1	-	-	2/12/26/26	0/6/6/6
2	B37	B	1	-	-	2/12/26/26	0/6/6/6
2	B37	A	1	-	-	2/12/26/26	0/6/6/6

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	B37	C38-N26	4.95	1.45	1.34
2	B	1	B37	C38-N26	4.95	1.45	1.34
2	A	1	B37	C3-C4	4.94	1.49	1.42
2	C	1	B37	C3-C4	4.86	1.49	1.42
2	A	1	B37	C38-N26	4.78	1.45	1.34
2	B	1	B37	C3-C4	4.57	1.49	1.42
2	A	1	B37	C43-N42	4.26	1.42	1.35
2	C	1	B37	C43-N42	4.26	1.42	1.35
2	A	1	B37	C40-C41	4.24	1.49	1.42
2	B	1	B37	C43-N42	4.19	1.42	1.35
2	C	1	B37	C40-C41	4.13	1.49	1.42
2	A	1	B37	C39-C40	3.91	1.50	1.43
2	B	1	B37	C40-C41	3.80	1.48	1.42
2	A	1	B37	C9-C10	3.68	1.46	1.37
2	B	1	B37	C44-C39	3.68	1.46	1.37
2	B	1	B37	C39-C40	3.66	1.49	1.43
2	C	1	B37	C39-C40	3.65	1.49	1.43
2	C	1	B37	C48-C49	3.63	1.45	1.36
2	A	1	B37	C2-C1	3.58	1.44	1.36
2	A	1	B37	C25-N26	3.55	1.53	1.47
2	C	1	B37	C47-C46	3.54	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	B37	C41-N42	3.54	1.41	1.35
2	C	1	B37	C9-C10	3.53	1.45	1.37
2	B	1	B37	C56-C55	3.51	1.44	1.36
2	C	1	B37	C56-C55	3.51	1.44	1.36
2	C	1	B37	C2-C1	3.49	1.44	1.36
2	B	1	B37	C11-C10	3.49	1.46	1.38
2	B	1	B37	C9-C10	3.47	1.45	1.37
2	A	1	B37	C56-C55	3.43	1.44	1.36
2	B	1	B37	C58-C59	3.40	1.44	1.36
2	B	1	B37	C25-N26	3.35	1.53	1.47
2	C	1	B37	C25-N26	3.34	1.53	1.47
2	A	1	B37	C47-C46	3.29	1.44	1.36
2	B	1	B37	C48-C49	3.27	1.44	1.36
2	B	1	B37	C47-C46	3.25	1.44	1.36
2	A	1	B37	C11-C10	3.23	1.45	1.38
2	B	1	B37	C2-C1	3.17	1.43	1.36
2	B	1	B37	C12-C11	3.13	1.43	1.36
2	A	1	B37	C48-C49	3.12	1.43	1.36
2	A	1	B37	C58-C59	3.02	1.43	1.36
2	A	1	B37	C44-C39	3.01	1.44	1.37
2	A	1	B37	C12-C11	3.01	1.42	1.36
2	C	1	B37	C11-C10	3.00	1.45	1.38
2	B	1	B37	C39-C38	2.91	1.55	1.50
2	B	1	B37	C41-N42	2.86	1.40	1.35
2	C	1	B37	C44-C39	2.86	1.44	1.37
2	A	1	B37	C41-N42	2.82	1.40	1.35
2	C	1	B37	C58-C59	2.78	1.43	1.36
2	A	1	B37	C6-N5	2.73	1.38	1.33
2	C	1	B37	C6-N5	2.73	1.38	1.33
2	C	1	B37	C12-C11	2.72	1.42	1.36
2	B	1	B37	C6-N5	2.62	1.38	1.33
2	A	1	B37	C39-C38	2.61	1.54	1.50
2	B	1	B37	C57-C56	2.43	1.44	1.38
2	C	1	B37	C49-C41	2.41	1.46	1.41
2	C	1	B37	C57-C56	2.40	1.44	1.38
2	A	1	B37	C57-C56	2.39	1.44	1.38
2	C	1	B37	C48-C47	2.35	1.44	1.38
2	A	1	B37	C48-C47	2.28	1.44	1.38
2	B	1	B37	C58-C57	2.24	1.44	1.38
2	C	1	B37	C58-C57	2.21	1.43	1.38
2	C	1	B37	C46-C40	2.20	1.46	1.42
2	B	1	B37	C48-C47	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B37	C58-C57	2.18	1.43	1.38
2	B	1	B37	C49-C41	2.11	1.45	1.41
2	A	1	B37	C28-C21	2.08	1.58	1.52
2	B	1	B37	C46-C40	2.03	1.46	1.42
2	A	1	B37	C27-N26	2.01	1.50	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	B37	C40-C41-N42	-5.92	117.81	123.35
2	A	1	B37	C40-C41-N42	-5.78	117.94	123.35
2	B	1	B37	C40-C41-N42	-5.59	118.11	123.35
2	B	1	B37	C43-N42-C41	5.35	125.41	117.86
2	A	1	B37	C43-N42-C41	5.17	125.14	117.86
2	C	1	B37	C43-N42-C41	4.94	124.82	117.86
2	A	1	B37	C44-C43-N42	-4.23	117.99	121.83
2	B	1	B37	C44-C43-N42	-4.12	118.09	121.83
2	C	1	B37	C44-C43-N42	-4.04	118.16	121.83
2	A	1	B37	C40-C39-C38	2.97	124.38	120.41
2	B	1	B37	C12-C4-N5	2.78	122.93	118.69
2	C	1	B37	C40-C39-C38	2.72	124.06	120.41
2	A	1	B37	C12-C4-N5	2.63	122.70	118.69
2	C	1	B37	C49-C41-N42	2.57	122.33	119.09
2	B	1	B37	C3-C4-N5	-2.55	118.46	122.26
2	C	1	B37	C12-C4-N5	2.54	122.57	118.69
2	A	1	B37	C3-C4-N5	-2.41	118.68	122.26
2	A	1	B37	C49-C41-N42	2.36	122.06	119.09
2	C	1	B37	C3-C4-N5	-2.31	118.83	122.26
2	B	1	B37	C49-C41-N42	2.21	121.87	119.09
2	A	1	B37	C55-C54-C59	-2.13	116.76	118.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	B37	O65-C38-N26-C25
2	C	1	B37	O65-C38-N26-C25
2	A	1	B37	O65-C38-N26-C25
2	B	1	B37	C9-C10-C20-C21
2	C	1	B37	C9-C10-C20-C21
2	A	1	B37	C9-C10-C20-C21

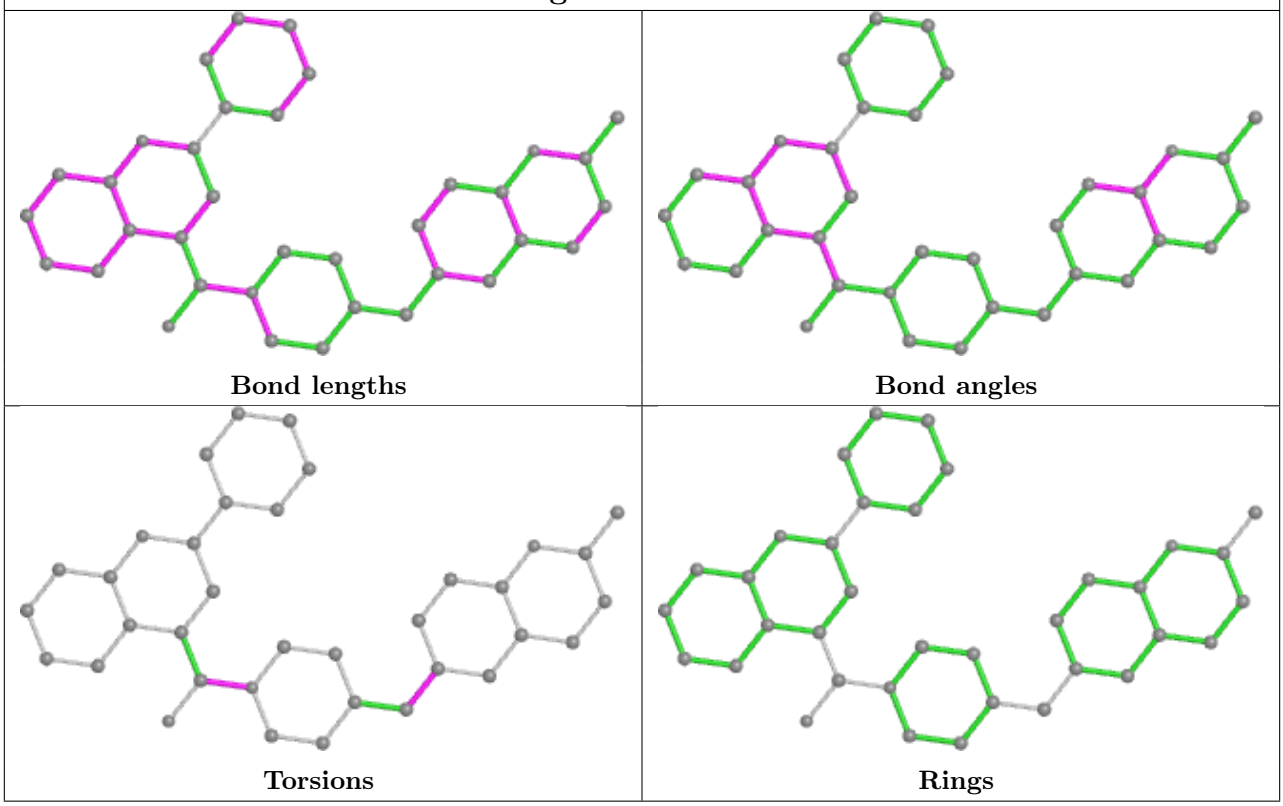
There are no ring outliers.

3 monomers are involved in 11 short contacts:

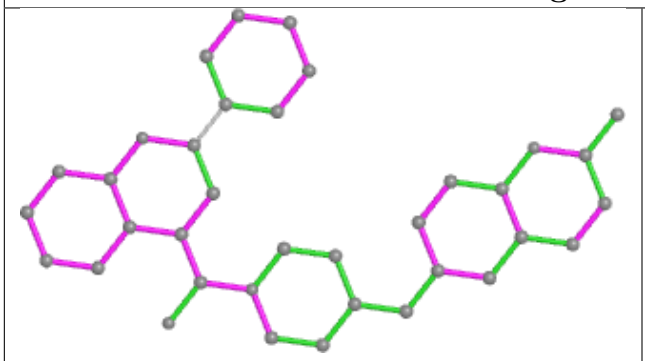
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	B37	2	0
2	B	1	B37	5	0
2	A	1	B37	4	0

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 then 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.

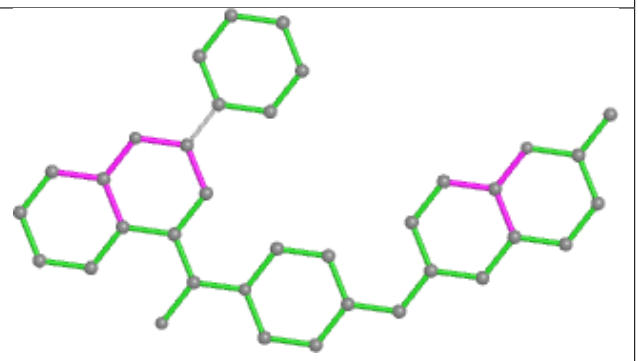
Ligand B37 C 1



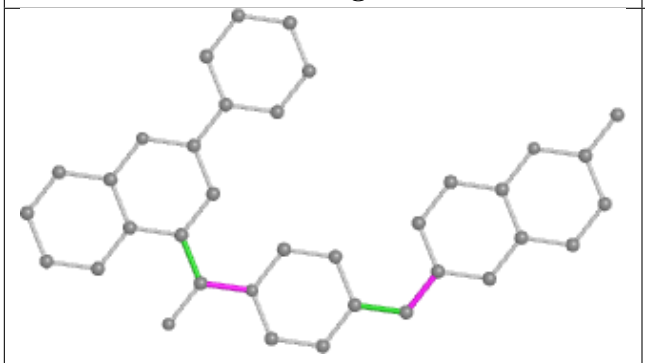
Ligand B37 B 1



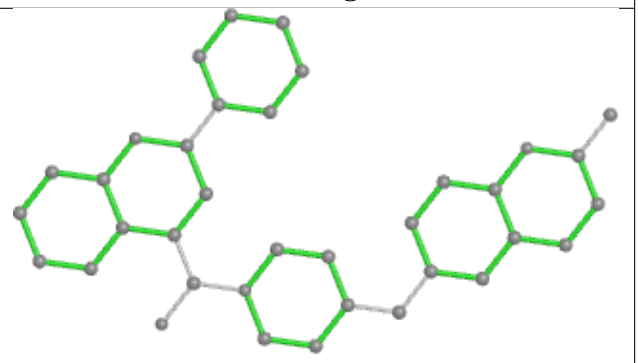
Bond lengths



Bond angles

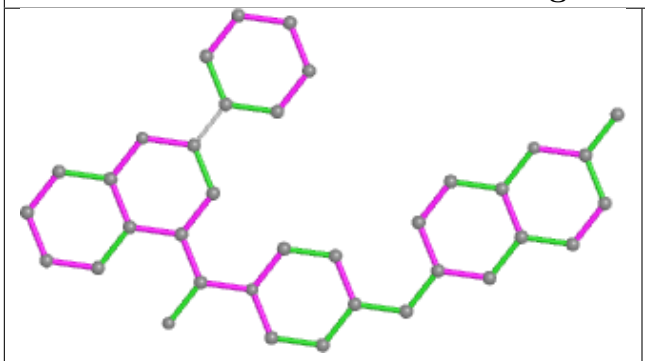


Torsions

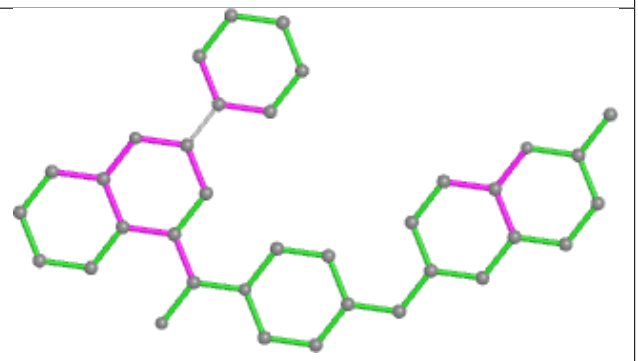


Rings

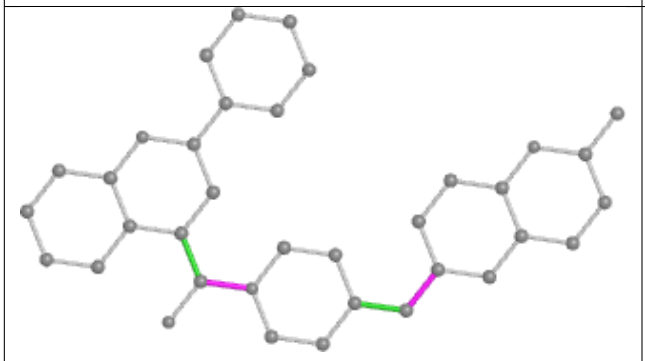
Ligand B37 A 1



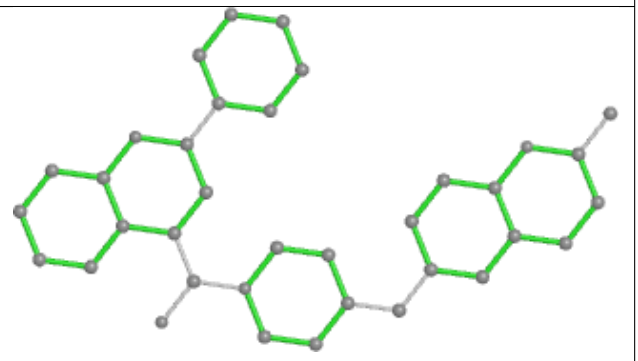
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	681/769 (88%)	0.28	48 (7%)	16	16	26, 41, 91, 126	0
1	B	675/769 (87%)	0.32	71 (10%)	6	6	26, 44, 99, 111	0
1	C	665/769 (86%)	0.34	60 (9%)	9	9	28, 44, 98, 121	0
All	All	2021/2307 (87%)	0.31	179 (8%)	9	9	26, 43, 95, 126	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	8.3
1	A	2195	ALA	8.2
1	A	2194	PHE	6.8
1	A	2047	LEU	6.5
1	C	1644	ASN	6.4
1	A	2143	VAL	6.4
1	B	2189	LEU	6.4
1	B	1682	ILE	5.7
1	A	1643	TRP	5.4
1	B	2041	LEU	5.2
1	B	2037	ARG	5.1
1	C	2086	TYR	5.1
1	A	2193	SER	5.0
1	B	1669	PHE	5.0
1	B	2143	VAL	5.0
1	A	1685	GLU	4.9
1	B	2082	LEU	4.8
1	A	2083	LEU	4.8
1	B	2083	LEU	4.7
1	C	1682	ILE	4.7
1	A	1683	ASN	4.7
1	B	2145	GLU	4.6
1	B	2085	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	1681	VAL	4.5
1	A	2191	LEU	4.5
1	B	2144	GLY	4.5
1	C	1679	ARG	4.5
1	B	1637	PRO	4.4
1	C	1685	GLU	4.4
1	A	1684	GLY	4.4
1	C	2144	GLY	4.3
1	C	2041	LEU	4.3
1	C	2082	LEU	4.3
1	B	2043	THR	4.3
1	A	2192	GLU	4.2
1	B	2086	TYR	4.2
1	C	1652	GLY	4.1
1	A	1682	ILE	4.1
1	B	1651	LYS	4.0
1	C	2142	GLN	4.0
1	A	1648	ASN	4.0
1	A	1911	ASN	4.0
1	A	1647	ALA	3.9
1	C	1668	LYS	3.8
1	A	1669	PHE	3.8
1	A	1668	LYS	3.7
1	A	2190	LYS	3.6
1	A	2037	ARG	3.5
1	A	1651	LYS	3.5
1	B	1681	VAL	3.5
1	B	2188	GLY	3.5
1	A	1838	ASP	3.4
1	C	2044	MET	3.4
1	B	1643	TRP	3.4
1	B	1685	GLU	3.4
1	A	2041	LEU	3.4
1	B	2142	GLN	3.4
1	C	1645	ASP	3.3
1	B	2146	ALA	3.3
1	A	1646	ALA	3.3
1	B	2187	LYS	3.2
1	C	1669	PHE	3.2
1	B	1645	ASP	3.2
1	A	1666	LEU	3.2
1	A	2145	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2144	GLY	3.2
1	B	1668	LYS	3.2
1	A	1681	VAL	3.1
1	A	2189	LEU	3.1
1	B	1838	ASP	3.1
1	C	1666	LEU	3.1
1	B	2047	LEU	3.1
1	B	2186	LEU	3.1
1	C	2037	ARG	3.0
1	B	1649	PRO	3.0
1	C	1649	PRO	3.0
1	C	1680	THR	3.0
1	C	1855	GLY	2.9
1	B	2179	TYR	2.9
1	C	2141	HIS	2.9
1	B	2134	TYR	2.9
1	C	1683	ASN	2.9
1	C	2085	ILE	2.9
1	C	2089	ILE	2.9
1	A	1679	ARG	2.9
1	A	2043	THR	2.9
1	A	1649	PRO	2.8
1	B	1636	VAL	2.8
1	B	2046	ARG	2.8
1	C	1911	ASN	2.8
1	A	1667	LYS	2.8
1	C	2047	LEU	2.8
1	B	1648	ASN	2.8
1	B	1911	ASN	2.8
1	C	2040	LEU	2.8
1	C	2083	LEU	2.8
1	A	2046	ARG	2.8
1	C	1655	TYR	2.8
1	A	2142	GLN	2.8
1	C	1663	MET	2.8
1	B	1667	LYS	2.7
1	C	2043	THR	2.7
1	B	2141	HIS	2.7
1	B	1666	LEU	2.7
1	A	1654	GLN	2.7
1	B	1647	ALA	2.7
1	B	1652	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1645	ASP	2.6
1	B	1679	ARG	2.6
1	C	1660	SER	2.6
1	C	2046	ARG	2.6
1	B	1642	ALA	2.6
1	B	2150	GLU	2.6
1	C	1664	GLU	2.6
1	C	1638	LEU	2.6
1	C	1643	TRP	2.6
1	B	2139	LEU	2.6
1	C	1653	PHE	2.6
1	B	1644	ASN	2.6
1	B	2044	MET	2.6
1	A	1655	TYR	2.6
1	C	1647	ALA	2.5
1	B	1655	TYR	2.5
1	B	1688	PHE	2.5
1	B	2036	ARG	2.5
1	B	1683	ASN	2.5
1	C	1665	THR	2.5
1	C	1913	ALA	2.5
1	A	1483	ILE	2.5
1	C	1688	PHE	2.5
1	C	1662	GLY	2.4
1	A	1664	GLU	2.4
1	C	1658	LEU	2.4
1	C	1670	ASP	2.4
1	B	1662	GLY	2.4
1	C	1932	THR	2.4
1	C	1639	PHE	2.4
1	B	2084	PRO	2.4
1	A	1853	GLU	2.4
1	C	1973	PHE	2.3
1	C	1686	GLU	2.3
1	B	1483	ILE	2.3
1	B	1680	THR	2.3
1	C	1661	GLU	2.3
1	B	2182	LEU	2.3
1	B	1492	TRP	2.3
1	B	1972	SER	2.3
1	C	1936	ILE	2.3
1	B	1973	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1651	LYS	2.2
1	B	1824	LYS	2.2
1	B	1933	ALA	2.2
1	A	1688	PHE	2.2
1	A	2040	LEU	2.2
1	C	1910	PRO	2.2
1	B	1687	ARG	2.2
1	B	2158	TRP	2.2
1	C	1659	THR	2.2
1	C	1977	ALA	2.1
1	A	2036	ARG	2.1
1	B	1912	SER	2.1
1	A	1687	ARG	2.1
1	C	2145	GLU	2.1
1	C	1974	ILE	2.1
1	B	1653	PHE	2.1
1	B	2152	ILE	2.1
1	C	1657	TYR	2.1
1	B	2040	LEU	2.1
1	B	1657	TYR	2.1
1	B	1932	THR	2.1
1	C	2186	LEU	2.1
1	B	1661	GLU	2.1
1	A	1641	VAL	2.1
1	C	2188	GLY	2.1
1	B	1684	GLY	2.0
1	B	1646	ALA	2.0
1	B	2183	ASP	2.0
1	A	2085	ILE	2.0
1	A	1973	PHE	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)

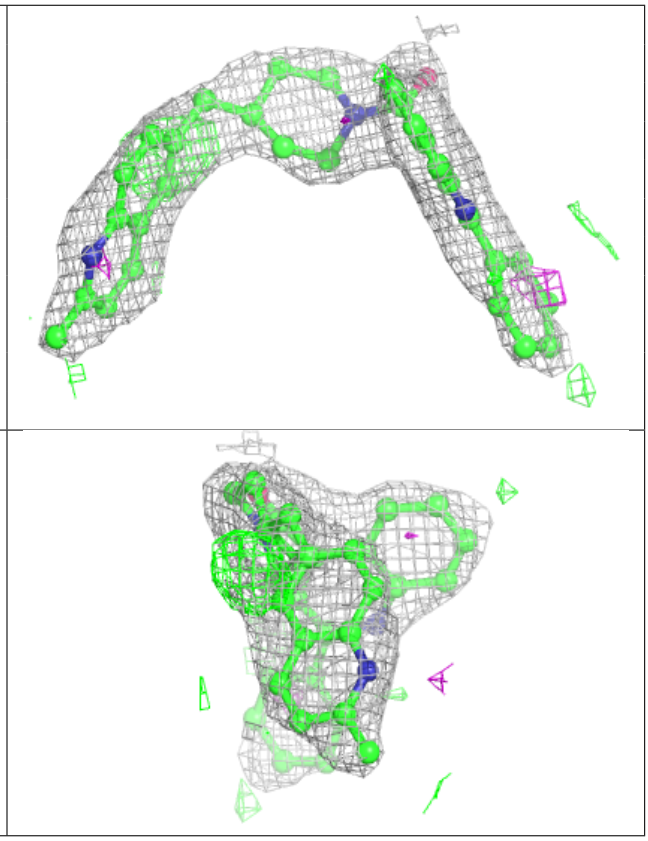
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B37	B	1	36/36	0.86	0.25	66,72,80,81	0
2	B37	A	1	36/36	0.87	0.21	61,66,77,78	0
2	B37	C	1	36/36	0.87	0.21	59,64,68,69	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.

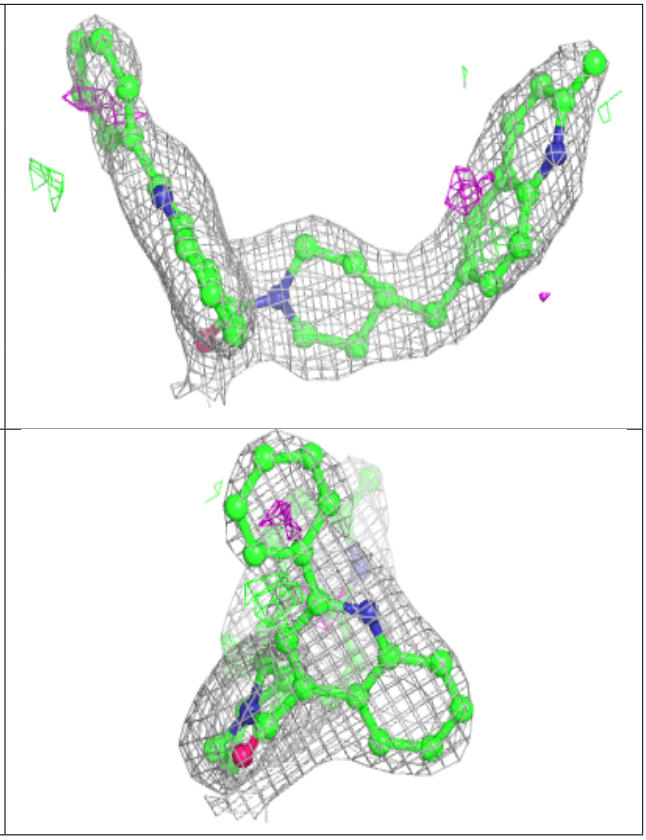
Electron density around B37 B 1:

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



Electron density around B37 A 1:

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



Electron density around B37 C 1:

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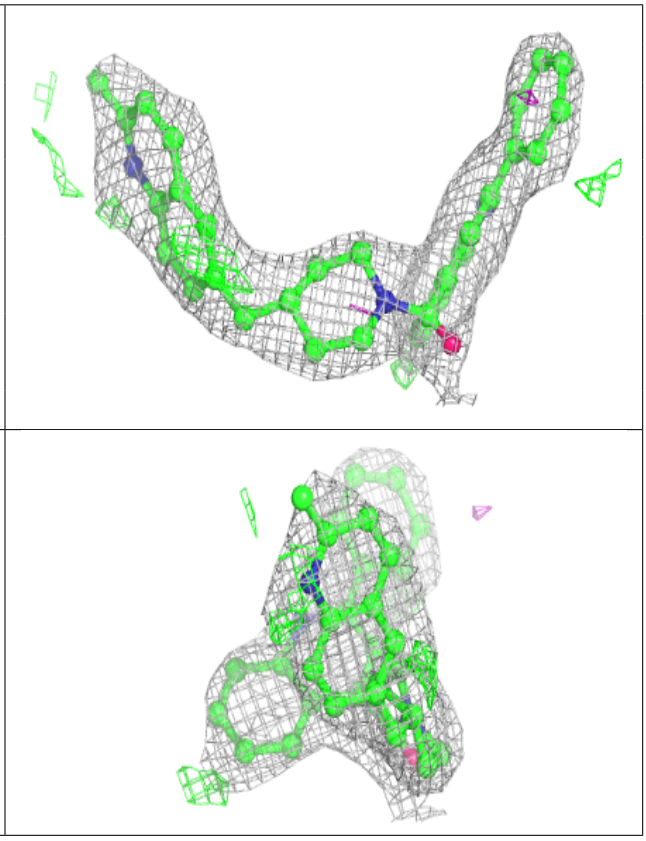
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.