Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:03 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

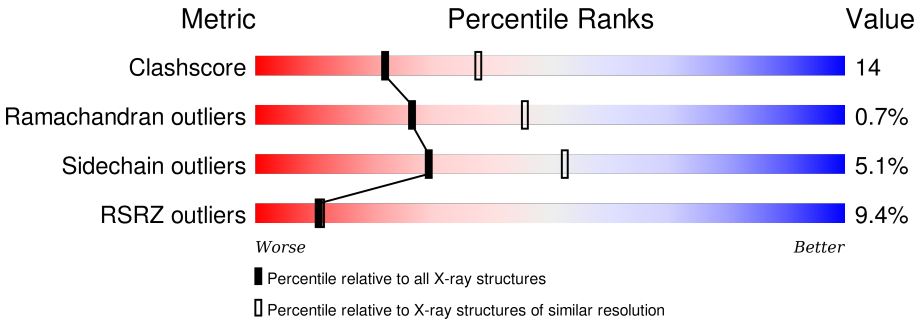
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	7% 65% 21% • 11%
1	B	769	10% 62% 23% • 12%
1	C	769	8% 62% 22% • 14%

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	B37	B	1	-	-	-	X

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
1	A	681	Total	C	N	O	S	0	0	0
			5424	3459	930	1016	19			
1	B	675	Total	C	N	O	S	0	0	0
			5376	3427	923	1007	19			
1	C	665	Total	C	N	O	S	0	0	0
			5298	3374	912	993	19			

There are 33 discrepancies between the modelled and reference sequences:

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

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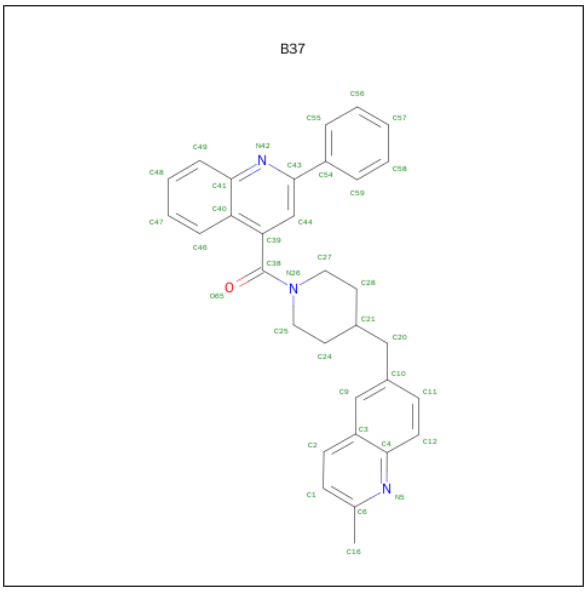
Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	EXPRESSION TAG	UNP Q00955
C	1475	SER	-	EXPRESSION TAG	UNP Q00955
C	2234	LEU	-	EXPRESSION TAG	UNP Q00955
C	2235	GLU	-	EXPRESSION TAG	UNP Q00955
C	2236	HIS	-	EXPRESSION TAG	UNP Q00955
C	2237	HIS	-	EXPRESSION TAG	UNP Q00955
C	2238	HIS	-	EXPRESSION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

- Molecule 2 is 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
2	A	1	Total C N O 36 32 3 1	0	0
2	B	1	Total C N O 36 32 3 1	0	0
2	C	1	Total C N O 36 32 3 1	0	0

- Molecule 3 is water.

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

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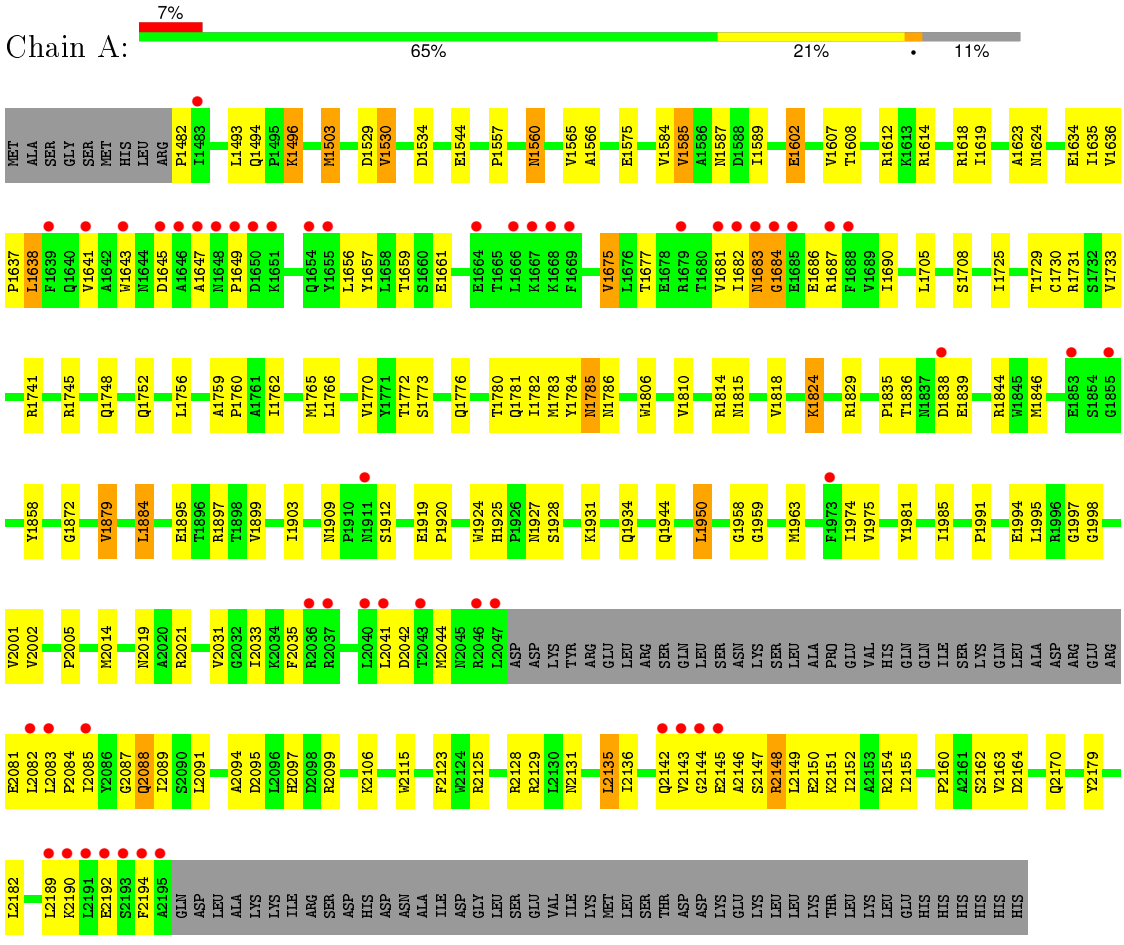
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	222	Total O 222 222	0	0
3	C	210	Total O 210 210	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

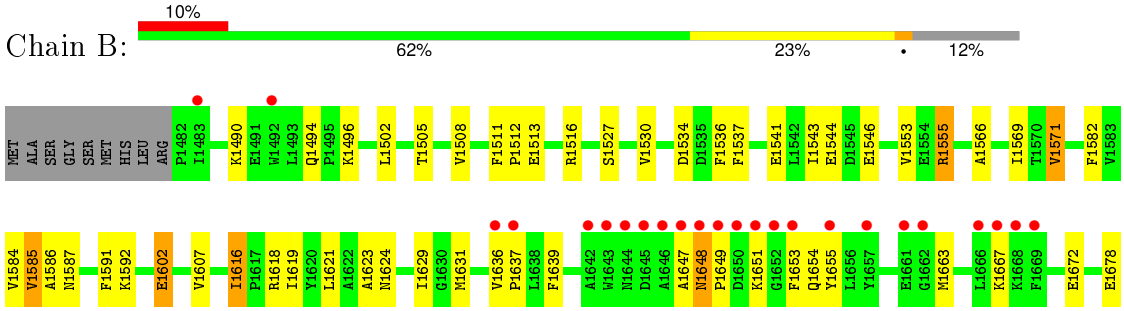
- Molecule 1: Acetyl-CoA carboxylase

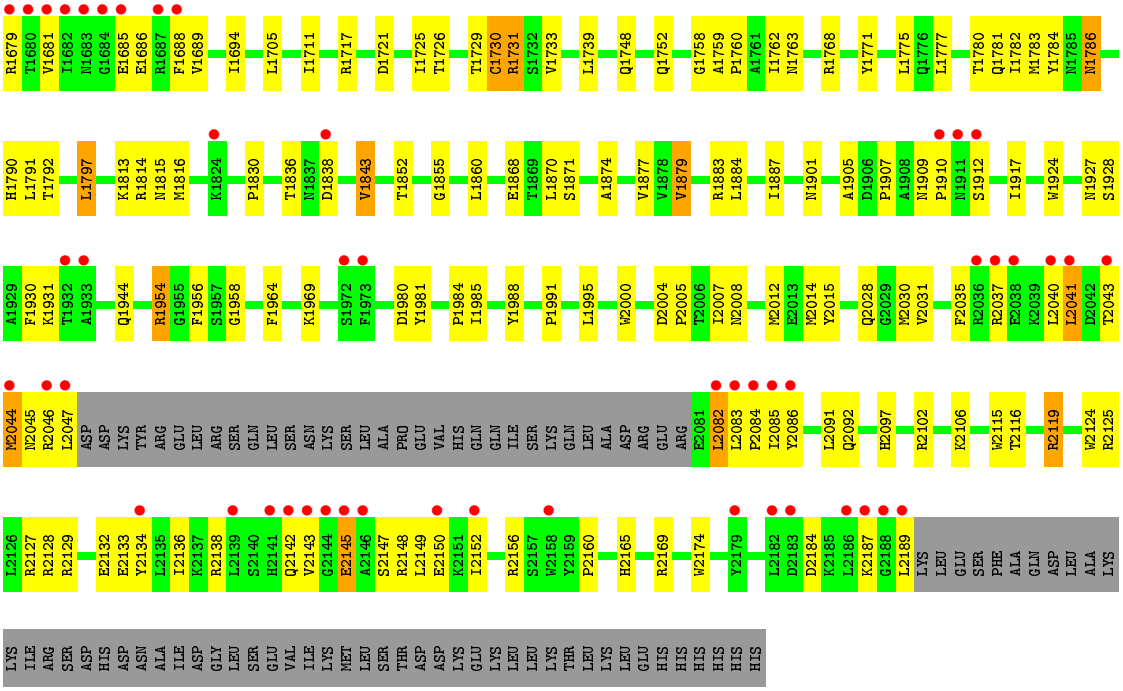
Chain A:



- Molecule 1: Acetyl-CoA carboxylase

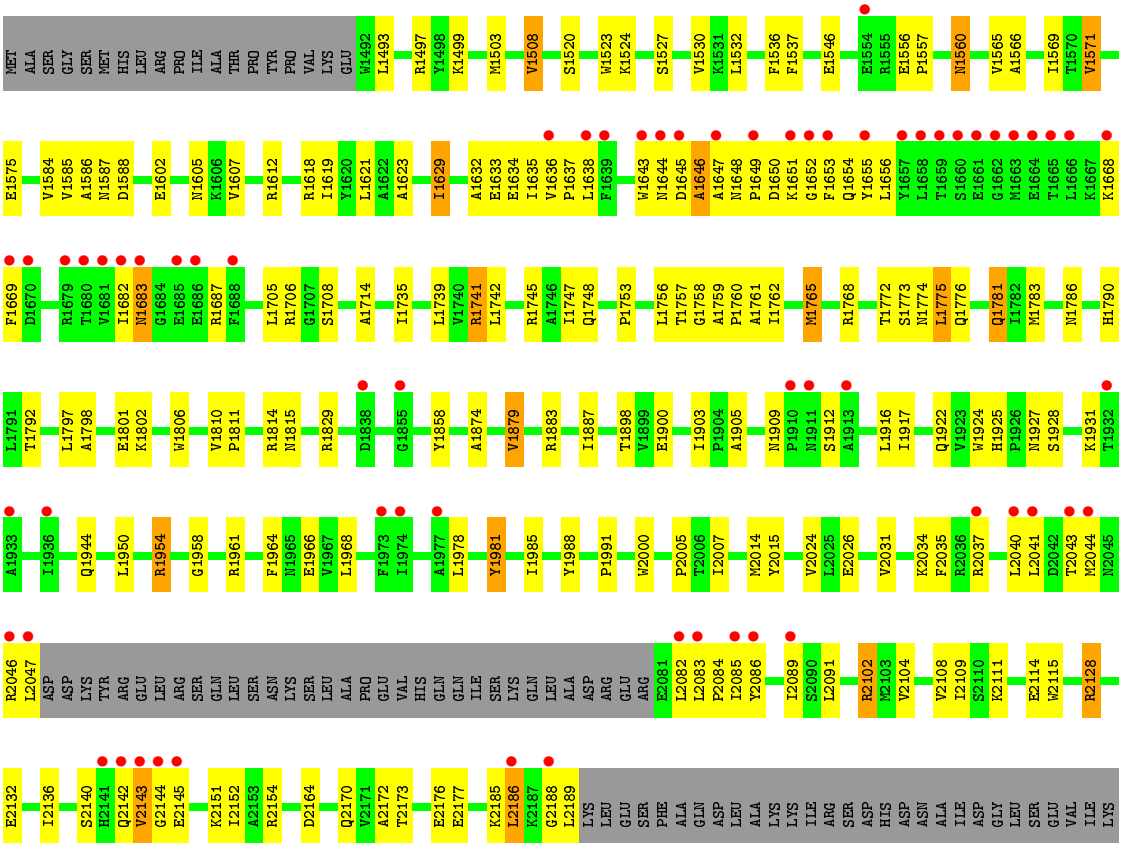
Chain B:





• Molecule 1: Acetyl-CoA carboxylase

Chain C:



MET
LEU
SER
THR
ASP
ASP
LYS
GLU
LYS
LEU
LEU
LYS
THR
LEU
LYS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

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]	4.40 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.233 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 146123 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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:HD22	1:A:1560:ASN:H	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:H	1:A:2082:LEU:HD23	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:2005:PRO:HG3	1:C:2014:MET:HB2	1.72	0.69
1:C:1646:ALA:C	1:C:1648:ASN:H	1.96	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:CD	1:A:1496:LYS:H	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:ND2	1:A:1560:ASN:H	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:C:1773:SER:N	1:C:1776:GLN:HE21	1.96	0.62
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.82	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:ND2	1:C:1560:ASN:H	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:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.02	0.56
1:A:1818:VAL:HG22	3:A:394:HOH:O	2.04	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:C:1790:HIS:HD2	3:C:64:HOH:O	1.89	0.55
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.87	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:2102:ARG:O	1:B:2106:LYS:HG2	2.06	0.55
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.72	0.55
1:C:1587:ASN:ND2	1:C:1623:ALA:H	2.04	0.55
1:C:1546:GLU:H	1:C:1546:GLU:CD	2.10	0.55
1:B:2083:LEU:HB2	1:B:2084:PRO:HD3	1.89	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:1905:ALA:HB1	1:C:1912:SER:OG	2.07	0.55
1:C:1556:GLU:HG3	1:C:1557:PRO:HD2	1.88	0.55
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.89	0.55
1:B:1585:VAL:CG1	1:B:1607:VAL:HG11	2.35	0.54
1:A:2031:VAL:HG11	1:A:2091:LEU:HD12	1.88	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:2185:LYS:O	1:C:2189:LEU:HD13	2.08	0.54
1:C:1647:ALA:O	1:C:1649:PRO:HD3	2.08	0.54
1:C:1637:PRO:HG2	1:C:1638:LEU:CD1	2.37	0.54
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.90	0.54
1:C:1643:TRP:CD1	1:C:1649:PRO:HA	2.43	0.54
1:B:1730:CYS:N	1:B:1752:GLN:HE21	2.05	0.54
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.73	0.54
1:B:1958:GLY:H	2:B:1:B37:C2	2.21	0.53
1:C:1759:ALA:N	1:C:1774:ASN:HD21	1.93	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: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: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:1643:TRP:HA	1:C:1653:PHE:HA	1.90	0.52
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	1.90	0.52
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.38	0.52
1:A:2142:GLN:HE22	1:A:2190:LYS:HG2	1.74	0.52
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.10	0.52
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.24	0.52
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.91	0.52
1:A:1838:ASP:O	1:A:1839:GLU:HG3	2.10	0.52
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.13	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:A:2095:ASP:O	1:A:2099:ARG:HD3	2.09	0.52
1:C:1560:ASN:N	1:C:1560:ASN:HD22	2.03	0.52
1:B:1729:THR:O	1:B:1730:CYS:HB3	2.10	0.52
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.91	0.51
1:B:2082:LEU:HD13	1:B:2086:TYR:CD1	2.45	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: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:B:1587:ASN:HB2	1:B:1623:ALA:O	2.10	0.51
1:A:2192:GLU:HG2	1:A:2192:GLU:O	2.10	0.51
1:A:1496:LYS:N	1:A:1496:LYS:HD3	2.25	0.51
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.93	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: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:C:1645:ASP:O	1:C:1646:ALA:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:GLN:CA	1:A:2088:GLN:HE21	2.23	0.50
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:B:2031:VAL:HG21	1:B:2091:LEU:HD12	1.93	0.50
1:C:1768:ARG:HH11	1:C:1768:ARG:HG2	1.77	0.50
1:C:1508:VAL:HG11	1:C:1565:VAL:CG2	2.42	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:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.93	0.50
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.29	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:A:1903:ILE:HD12	1:A:1903:ILE:N	2.26	0.50
1:C:1958:GLY:H	2:C:1:B37:C2	2.25	0.50
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.74	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:B:1786:ASN:ND2	1:C:1964:PHE:O	2.41	0.49
1:A:1785:ASN:HD22	1:A:1785:ASN:N	2.10	0.49
1:A:2106:LYS:HA	1:A:2106:LYS:HE2	1.93	0.49
1:C:2047:LEU:HD13	1:C:2047:LEU:C	2.32	0.49
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.94	0.49
1:A:1974:ILE:HB	1:A:2002:VAL:HG21	1.93	0.49
1:B:2156:ARG:HH11	1:B:2156:ARG:HG3	1.77	0.49
1:B:1653:PHE:CZ	1:C:2089:ILE:HD13	2.48	0.49
1:B:1901:ASN:HB3	1:B:1917:ILE:HB	1.93	0.49
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.13	0.49
1:B:1775:LEU:O	1:B:1781:GLN:NE2	2.42	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:B:2043:THR:C	1:B:2045:ASN:H	2.16	0.48
1:A:1909:ASN:ND2	1:A:1912:SER:HB3	2.28	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:C:2031:VAL:HG21	1:C:2091:LEU:HD23	1.95	0.48
1:B:2030:MET:HE3	1:B:2030:MET:HA	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:C:2143:VAL:HG23	1:C:2143:VAL:O	2.13	0.47
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.44	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:C:1633:GLU:HA	1:C:1636:VAL:HG23	1.97	0.47
1:C:1632:ALA:HB1	1:C:1634:GLU:OE2	2.14	0.47
1:C:2142:GLN:NE2	1:C:2189:LEU:HB2	2.30	0.47
1:B:2124:TRP:CE3	1:B:2169:ARG:HA	2.49	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:C:2142:GLN:O	1:C:2144:GLY:N	2.48	0.47
1:A:2147:SER:OG	1:A:2150:GLU:HG3	2.15	0.47
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.96	0.47
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.45	0.47
1:A:2041:LEU:HA	1:A:2044:MET:CG	2.44	0.47
1:A:2033:ILE:HD11	2:A:1:B37:H58	1.95	0.47
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.97	0.47
1:C:1635:ILE:O	1:C:1635:ILE:HG22	2.14	0.47
3:B:683:HOH:O	1:C:1765:MET:HE2	2.14	0.47
1:B:1544:GLU:OE2	1:B:1602:GLU:OE1	2.33	0.46
1:C:1768:ARG:NH1	1:C:1768:ARG:HG2	2.30	0.46
1:C:1520:SER:O	1:C:1524:LYS:HG2	2.14	0.46
1:C:2041:LEU:HA	1:C:2044:MET:HG2	1.97	0.46
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.97	0.46
1:C:2172:ALA:O	1:C:2176:GLU:HG3	2.16	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
1:B:1909:ASN:HD22	1:B:1912:SER:HB2	1.80	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:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.98	0.46
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.16	0.46
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.31	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:1560:ASN:ND2	1:A:1560:ASN:N	2.62	0.46
1:A:1529:ASP:O	1:A:1530:VAL:C	2.53	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:2147:SER:HB3	1:B:2150:GLU:HG3	1.99	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:C:1560:ASN:N	1:C:1560:ASN:ND2	2.61	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:1772:THR:N	1:C:1776:GLN:HE22	1.97	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: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:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.98	0.45
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.81	0.45
1:C:2085:ILE:HG23	1:C:2086:TYR:HD1	1.81	0.45
1:C:1629:ILE:H	1:C:1629:ILE:HD13	1.81	0.45
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.16	0.45
1:B:2134:TYR:CE1	1:B:2138:ARG:HD2	2.51	0.45
1:A:1503:MET:CE	1:A:1589:ILE:HG13	2.46	0.45
1:C:1646:ALA:C	1:C:1648:ASN:N	2.64	0.45
1:B:1909:ASN:ND2	1:B:1912:SER:N	2.65	0.45
1:A:1496:LYS:N	1:A:1496:LYS:CD	2.79	0.45
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	1.99	0.45
1:C:1523:TRP:HB3	1:C:1530:VAL:HG21	1.97	0.45
1:A:1705:LEU:O	1:A:1708:SER:HB3	2.16	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:1903:ILE:HG12	1:C:1917:ILE:HD13	1.98	0.44
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.18	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: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:1639:PHE:O	1:C:2046:ARG:NH1	2.51	0.44
1:B:1679:ARG:HG3	1:B:1679:ARG:O	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:2082:LEU:O	1:A:2085:ILE:HG22	2.19	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:B:1653:PHE:CD1	1:B:1653:PHE:N	2.86	0.43
1:A:1998:GLY:HA3	3:A:3:HOH:O	2.18	0.43
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.84	0.43
1:B:2132:GLU:O	1:B:2136:ILE:HG13	2.19	0.43
1:B:1964:PHE:O	1:C:1786:ASN:OD1	2.36	0.43
1:B:1813:LYS:HG2	1:B:1816:MET:SD	2.59	0.43
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.00	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:1681:VAL:HA	1:B:1685:GLU:O	2.18	0.43
1:A:2082:LEU:N	1:A:2082:LEU:HD23	2.30	0.43
1:C:2083:LEU:HB2	1:C:2084:PRO:HD3	2.01	0.43
1:A:1482:PRO:N	3:A:88:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1753:PRO:HB3	1:C:1775:LEU:HD12	1.99	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:HA	1:C:2186:LEU:HD12	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:C:1499:LYS:O	1:C:1503:MET:HG2	2.19	0.42
1:B:1530:VAL:HG13	1:B:1530:VAL: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:B:1988:TYR:HA	1:B:2015:TYR:O	2.19	0.42
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.50	0.42
2:B:1:B37:C55	1:C:1761:ALA:HA	2.50	0.42
1:B:1586:ALA:CB	1:B:1621:LEU:HB2	2.49	0.42
1:C:2083:LEU:N	1:C:2083:LEU:HD12	2.35	0.42
1:A:1920:PRO:HD2	1:A:1925:HIS:CE1	2.54	0.42
1:B:1649:PRO:C	1:B:1651:LYS:H	2.23	0.42
1:A:1835:PRO:HG3	1:A:1846:MET:SD	2.59	0.42
1:C:2082:LEU:HA	1:C:2082:LEU:HD23	1.83	0.42
1:C:1927:ASN:OD1	1:C:1928:SER:N	2.51	0.42
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.18	0.42
1:B:1490:LYS:NZ	3:B:122:HOH:O	2.53	0.42
1:A:2094:ALA:HA	1:A:2097:HIS:HD2	1.85	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:B:1909:ASN:HA	1:B:1910:PRO:HD3	1.88	0.42
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	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:2189:LEU:HD12	1:A:2189:LEU:HA	1.79	0.41
1:A:1958:GLY:H	2:A:1:B37:H2	1.82	0.41
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.20	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:2189:LEU:N	1:C:2189:LEU:HD12	2.34	0.41
1:C:1575:GLU:HG2	3:C:56:HOH:O	2.20	0.41
1:A:2162:SER:HG	1:B:1797:LEU:HB3	1.84	0.41
1:B:1786:ASN:HA	1:B:1786:ASN:HD22	1.54	0.41
1:B:2037:ARG:NH1	1:B:2041:LEU:HD21	2.35	0.41
1:C:1917:ILE:HD12	1:C:1917:ILE:N	2.36	0.41
1:C:1810:VAL:HA	1:C:1811:PRO:HD3	1.96	0.41
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.53	0.41
1:B:2047:LEU:HD13	1:B:2047:LEU:C	2.41	0.41
1:C:1619:ILE:N	1:C:1619:ILE:HD12	2.35	0.41
1:A:1638:LEU:N	1:A:1638:LEU:HD23	2.36	0.41
1:B:1729:THR:HG23	1:B:1729:THR:O	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:1721:ASP:OD2	1:B:1814:ARG:NH1	2.52	0.41
1:C:1747:ILE:HD13	1:C:1802:LYS:CB	2.49	0.41
1:B:1511:PHE:N	1:B:1512:PRO:CD	2.84	0.41
1:C:2154:ARG:HH11	1:C:2154:ARG:HG3	1.84	0.41
1:B:1954:ARG:NH1	2:B:1:B37:H11	2.36	0.41
1:B:1663:MET:HG3	1:B:1688:PHE:CD2	2.55	0.41
1:C:2041:LEU:O	1:C:2044:MET:HB2	2.20	0.41
1:B:2000:TRP:CG	1:C:1705:LEU:HB3	2.56	0.41
1:B:1995:LEU:HA	1:B:1995:LEU:HD12	1.92	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:C:1774:ASN:HD22	1:C:1774:ASN:HA	1.67	0.41
1:B:1705:LEU:HB3	1:C:2000:TRP:CG	2.56	0.41
1:C:2154:ARG:NH1	1:C:2154:ARG:HG3	2.35	0.41
1:C:1605:ASN:ND2	1:C:1714:ALA:HB2	2.36	0.41
1:B:2149:LEU:HD13	1:B:2149:LEU:C	2.41	0.41
1:A:1614:ARG:HG3	1:A:1614:ARG:NH1	2.36	0.40
1:B:1629:ILE:HG22	1:C:2024:VAL:HB	2.03	0.40
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	2.03	0.40
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.51	0.40
1:B:2148:ARG:O	1:B:2152:ILE:HG13	2.20	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:A:1814:ARG:O	1:A:1815:ASN:HB2	2.21	0.40
1:B:2119:ARG:HB3	3:B:77:HOH:O	2.21	0.40
1:C:1954:ARG:HG2	1:C:1954:ARG:H	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.54	0.40
1:C:1900:GLU:HB3	1:C:1916:LEU:HD11	2.03	0.40
1:A:1659:THR:OG1	1:A:1661:GLU:HB3	2.22	0.40
1:B:2082:LEU:C	1:B:2082:LEU:HD12	2.41	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: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%)	21	37
1	B	671/769 (87%)	627 (93%)	39 (6%)	5 (1%)	26	46
1	C	661/769 (86%)	622 (94%)	35 (5%)	4 (1%)	30	50
All	All	2009/2307 (87%)	1885 (94%)	109 (5%)	15 (1%)	26	46

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

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%)	31 55
1	B	572/658 (87%)	539 (94%)	33 (6%)	25 45
1	C	563/658 (86%)	536 (95%)	27 (5%)	31 55
All	All	1712/1974 (87%)	1624 (95%)	88 (5%)	29 52

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

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	B37	A	1	-	41,41,41	2.68	24 (58%)	58,58,58	1.98	9 (15%)
2	B37	B	1	-	41,41,41	2.70	26 (63%)	58,58,58	1.92	6 (10%)
2	B37	C	1	-	41,41,41	2.66	26 (63%)	58,58,58	1.92	8 (13%)

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	A	1	-	-	0/16/26/26	0/6/6/6
2	B37	B	1	-	-	0/16/26/26	0/6/6/6
2	B37	C	1	-	-	0/16/26/26	0/6/6/6

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	B37	C58-C59	2.00	1.43	1.38
2	B	1	B37	C49-C41	2.01	1.45	1.41
2	B	1	B37	C28-C21	2.01	1.57	1.52
2	B	1	B37	C55-C54	2.04	1.43	1.39
2	B	1	B37	C46-C40	2.06	1.46	1.42
2	C	1	B37	C27-N26	2.06	1.50	1.47
2	C	1	B37	C28-C21	2.06	1.58	1.52
2	A	1	B37	C44-C43	2.07	1.42	1.39
2	A	1	B37	C27-N26	2.08	1.50	1.47
2	C	1	B37	C41-N42	2.08	1.41	1.37
2	C	1	B37	C55-C54	2.09	1.43	1.39
2	A	1	B37	C28-C21	2.17	1.58	1.52
2	C	1	B37	C46-C40	2.24	1.46	1.42
2	A	1	B37	C58-C57	2.24	1.43	1.38
2	B	1	B37	C48-C47	2.26	1.43	1.38
2	C	1	B37	C58-C57	2.27	1.43	1.38
2	A	1	B37	C58-C59	2.27	1.43	1.38
2	C	1	B37	C49-C41	2.30	1.46	1.41
2	B	1	B37	C58-C57	2.31	1.44	1.38
2	A	1	B37	C48-C47	2.35	1.44	1.38
2	C	1	B37	C48-C47	2.42	1.44	1.38
2	A	1	B37	C39-C38	2.45	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B37	C57-C56	2.47	1.44	1.38
2	C	1	B37	C57-C56	2.47	1.44	1.38
2	B	1	B37	C6-N5	2.49	1.38	1.33
2	B	1	B37	C57-C56	2.51	1.44	1.38
2	C	1	B37	C6-N5	2.59	1.38	1.33
2	A	1	B37	C6-N5	2.59	1.38	1.33
2	B	1	B37	C59-C54	2.62	1.44	1.39
2	C	1	B37	C59-C54	2.66	1.45	1.39
2	B	1	B37	C58-C59	2.70	1.44	1.38
2	C	1	B37	C12-C11	2.72	1.42	1.36
2	A	1	B37	C56-C55	2.73	1.44	1.38
2	B	1	B37	C39-C38	2.73	1.55	1.50
2	C	1	B37	C56-C55	2.82	1.44	1.38
2	B	1	B37	C56-C55	2.82	1.44	1.38
2	C	1	B37	C44-C39	2.91	1.44	1.37
2	A	1	B37	C59-C54	2.96	1.45	1.39
2	A	1	B37	C12-C11	3.00	1.42	1.36
2	C	1	B37	C11-C10	3.05	1.45	1.38
2	A	1	B37	C44-C39	3.08	1.44	1.37
2	A	1	B37	C48-C49	3.12	1.43	1.36
2	B	1	B37	C12-C11	3.12	1.43	1.36
2	B	1	B37	C2-C1	3.16	1.43	1.36
2	B	1	B37	C47-C46	3.24	1.44	1.36
2	B	1	B37	C48-C49	3.27	1.44	1.36
2	A	1	B37	C47-C46	3.28	1.44	1.36
2	A	1	B37	C11-C10	3.29	1.45	1.38
2	B	1	B37	C9-C10	3.35	1.45	1.37
2	C	1	B37	C9-C10	3.41	1.45	1.37
2	C	1	B37	C25-N26	3.44	1.53	1.47
2	B	1	B37	C25-N26	3.45	1.53	1.47
2	C	1	B37	C2-C1	3.48	1.44	1.36
2	B	1	B37	C44-C43	3.48	1.44	1.39
2	C	1	B37	C47-C46	3.54	1.44	1.36
2	A	1	B37	C9-C10	3.55	1.46	1.37
2	B	1	B37	C11-C10	3.56	1.46	1.38
2	A	1	B37	C2-C1	3.57	1.44	1.36
2	C	1	B37	C48-C49	3.62	1.45	1.36
2	A	1	B37	C25-N26	3.65	1.53	1.47
2	C	1	B37	C39-C40	3.75	1.49	1.43
2	B	1	B37	C39-C40	3.75	1.49	1.43
2	B	1	B37	C44-C39	3.82	1.46	1.37
2	A	1	B37	C39-C40	4.01	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	B37	C40-C41	4.02	1.48	1.42
2	C	1	B37	C40-C41	4.38	1.49	1.42
2	A	1	B37	C40-C41	4.50	1.49	1.42
2	A	1	B37	C38-N26	4.59	1.45	1.34
2	B	1	B37	C38-N26	4.75	1.45	1.34
2	C	1	B37	C38-N26	4.76	1.45	1.34
2	B	1	B37	C3-C4	5.02	1.49	1.42
2	B	1	B37	C43-N42	5.09	1.42	1.33
2	C	1	B37	C43-N42	5.15	1.42	1.33
2	A	1	B37	C43-N42	5.16	1.42	1.33
2	C	1	B37	C3-C4	5.33	1.49	1.42
2	A	1	B37	C3-C4	5.41	1.49	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	B37	C44-C43-N42	-5.37	117.99	122.24
2	B	1	B37	C44-C43-N42	-5.25	118.09	122.24
2	C	1	B37	C40-C41-N42	-5.22	117.81	122.90
2	C	1	B37	C44-C43-N42	-5.16	118.16	122.24
2	A	1	B37	C40-C41-N42	-5.09	117.94	122.90
2	B	1	B37	C40-C41-N42	-4.90	118.11	122.90
2	B	1	B37	C3-C4-N5	-2.19	118.46	122.25
2	A	1	B37	O65-C38-N26	-2.13	119.03	122.42
2	A	1	B37	C3-C4-N5	-2.07	118.68	122.25
2	C	1	B37	C10-C20-C21	2.04	117.71	114.62
2	A	1	B37	C49-C41-N42	2.10	122.06	118.73
2	C	1	B37	C39-C44-C43	2.17	122.04	120.68
2	C	1	B37	C49-C41-N42	2.27	122.33	118.73
2	A	1	B37	C39-C44-C43	2.39	122.18	120.68
2	C	1	B37	C12-C4-N5	2.42	122.57	118.73
2	A	1	B37	C12-C4-N5	2.50	122.70	118.73
2	B	1	B37	C12-C4-N5	2.64	122.93	118.73
2	B	1	B37	C44-C43-C54	2.95	125.81	121.89
2	C	1	B37	C40-C39-C38	3.14	124.06	120.38
2	A	1	B37	C40-C39-C38	3.42	124.38	120.38
2	C	1	B37	C43-N42-C41	9.18	124.82	118.00
2	A	1	B37	C43-N42-C41	9.62	125.14	118.00
2	B	1	B37	C43-N42-C41	9.97	125.41	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.35	52 (7%) 17 18	26, 41, 91, 126	0
1	B	675/769 (87%)	0.39	74 (10%) 7 7	26, 44, 99, 111	0
1	C	665/769 (86%)	0.40	64 (9%) 10 11	28, 44, 98, 121	0
All	All	2021/2307 (87%)	0.38	190 (9%) 11 11	26, 43, 95, 126	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	8.6
1	A	2195	ALA	8.5
1	A	2194	PHE	7.0
1	A	2047	LEU	6.8
1	C	1644	ASN	6.7
1	A	2143	VAL	6.7
1	B	2189	LEU	6.6
1	B	1682	ILE	6.0
1	A	1643	TRP	5.6
1	B	2041	LEU	5.4
1	B	2037	ARG	5.3
1	B	2143	VAL	5.2
1	C	2086	TYR	5.2
1	A	2193	SER	5.2
1	B	1669	PHE	5.2
1	A	1685	GLU	5.1
1	B	2082	LEU	5.0
1	A	2083	LEU	5.0
1	B	2083	LEU	4.9
1	C	1682	ILE	4.9
1	A	1683	ASN	4.9
1	B	2145	GLU	4.8
1	C	1681	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	2085	ILE	4.7
1	A	2191	LEU	4.7
1	B	2144	GLY	4.7
1	B	1637	PRO	4.7
1	C	1679	ARG	4.6
1	A	1684	GLY	4.6
1	C	2144	GLY	4.6
1	C	1685	GLU	4.6
1	C	2041	LEU	4.5
1	B	2043	THR	4.5
1	C	2082	LEU	4.4
1	A	2192	GLU	4.4
1	C	1652	GLY	4.4
1	B	2086	TYR	4.3
1	A	1682	ILE	4.3
1	C	2142	GLN	4.2
1	A	1647	ALA	4.2
1	B	1651	LYS	4.2
1	A	1648	ASN	4.2
1	A	1911	ASN	4.1
1	C	1668	LYS	3.9
1	A	1669	PHE	3.9
1	A	1668	LYS	3.8
1	B	1681	VAL	3.7
1	A	2190	LYS	3.7
1	A	2037	ARG	3.7
1	B	2188	GLY	3.7
1	A	1651	LYS	3.7
1	C	2044	MET	3.6
1	A	1838	ASP	3.6
1	B	1685	GLU	3.5
1	B	1643	TRP	3.5
1	A	2041	LEU	3.5
1	B	2142	GLN	3.5
1	B	2146	ALA	3.5
1	C	1645	ASP	3.5
1	A	1646	ALA	3.4
1	B	1645	ASP	3.4
1	B	2187	LYS	3.4
1	A	2144	GLY	3.4
1	A	2145	GLU	3.3
1	A	1666	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1681	VAL	3.3
1	C	1669	PHE	3.3
1	B	1838	ASP	3.3
1	B	1668	LYS	3.3
1	A	2189	LEU	3.3
1	B	2047	LEU	3.3
1	B	2186	LEU	3.2
1	C	1666	LEU	3.2
1	B	1649	PRO	3.2
1	C	1649	PRO	3.2
1	C	2037	ARG	3.2
1	C	1855	GLY	3.1
1	C	1680	THR	3.1
1	C	1683	ASN	3.1
1	B	2179	TYR	3.0
1	C	2141	HIS	3.0
1	A	2043	THR	3.0
1	A	1649	PRO	3.0
1	B	2134	TYR	3.0
1	C	2085	ILE	3.0
1	B	1636	VAL	3.0
1	C	2089	ILE	3.0
1	C	2047	LEU	3.0
1	A	1679	ARG	3.0
1	C	1663	MET	2.9
1	C	2083	LEU	2.9
1	B	2046	ARG	2.9
1	B	1648	ASN	2.9
1	B	1911	ASN	2.9
1	C	1911	ASN	2.9
1	A	1667	LYS	2.9
1	C	2040	LEU	2.9
1	A	2142	GLN	2.9
1	C	1655	TYR	2.9
1	C	2043	THR	2.9
1	A	2046	ARG	2.9
1	B	1647	ALA	2.9
1	B	1667	LYS	2.9
1	A	1654	GLN	2.8
1	B	1666	LEU	2.8
1	B	2141	HIS	2.8
1	B	1652	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1645	ASP	2.8
1	B	1642	ALA	2.8
1	B	1679	ARG	2.8
1	C	2046	ARG	2.8
1	C	1660	SER	2.8
1	B	2150	GLU	2.7
1	C	1664	GLU	2.7
1	C	1638	LEU	2.7
1	B	2044	MET	2.7
1	C	1647	ALA	2.7
1	C	1643	TRP	2.7
1	B	1644	ASN	2.7
1	B	2139	LEU	2.7
1	C	1653	PHE	2.7
1	A	1655	TYR	2.7
1	C	1665	THR	2.6
1	B	1655	TYR	2.6
1	B	2036	ARG	2.6
1	B	1688	PHE	2.6
1	C	1913	ALA	2.6
1	A	1483	ILE	2.6
1	C	1662	GLY	2.6
1	B	1683	ASN	2.6
1	C	1670	ASP	2.6
1	C	1688	PHE	2.6
1	C	1932	THR	2.5
1	B	1662	GLY	2.5
1	A	1664	GLU	2.5
1	C	1658	LEU	2.5
1	B	2084	PRO	2.5
1	A	1853	GLU	2.5
1	C	1639	PHE	2.5
1	C	1973	PHE	2.5
1	C	1686	GLU	2.4
1	B	1483	ILE	2.4
1	B	2182	LEU	2.4
1	B	1680	THR	2.4
1	C	1936	ILE	2.4
1	C	1661	GLU	2.4
1	B	1933	ALA	2.4
1	B	1972	SER	2.4
1	B	1973	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1492	TRP	2.4
1	C	1651	LYS	2.3
1	B	1824	LYS	2.3
1	A	1688	PHE	2.3
1	C	1659	THR	2.3
1	A	2040	LEU	2.3
1	C	1910	PRO	2.3
1	B	2158	TRP	2.3
1	C	1977	ALA	2.3
1	A	2036	ARG	2.3
1	B	1687	ARG	2.3
1	C	1974	ILE	2.2
1	C	2145	GLU	2.2
1	A	1687	ARG	2.2
1	B	2152	ILE	2.2
1	B	1912	SER	2.2
1	B	1653	PHE	2.2
1	C	1657	TYR	2.2
1	C	2188	GLY	2.2
1	C	2186	LEU	2.2
1	B	1932	THR	2.2
1	A	1641	VAL	2.2
1	B	1657	TYR	2.2
1	B	2040	LEU	2.2
1	B	1661	GLU	2.2
1	B	2183	ASP	2.2
1	B	1646	ALA	2.2
1	B	1684	GLY	2.2
1	C	1933	ALA	2.1
1	A	2085	ILE	2.1
1	A	1650	ASP	2.1
1	A	1973	PHE	2.1
1	A	1855	GLY	2.1
1	C	1838	ASP	2.1
1	C	1554	GLU	2.1
1	C	1636	VAL	2.0
1	B	1910	PRO	2.0
1	B	1650	ASP	2.0
1	B	2038	GLU	2.0
1	A	2082	LEU	2.0
1	A	1639	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	B37	B	1	36/36	0.86	0.25	2.13	66,72,80,81	0
2	B37	C	1	36/36	0.87	0.21	1.38	59,64,68,69	0
2	B37	A	1	36/36	0.87	0.21	1.37	61,66,77,78	0

6.5 Other polymers (i)

There are no such residues in this entry.