



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:30 am BST

PDB ID : 4ASI  
Title : Crystal structure of human ACACA C-terminal domain  
Authors : Froese, D.S.; Muniz, J.R.C.; Kiyani, W.; Krojer, T.; Vollmar, M.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Oppermann, U.; Yue, W.W.  
Deposited on : 2012-05-01  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

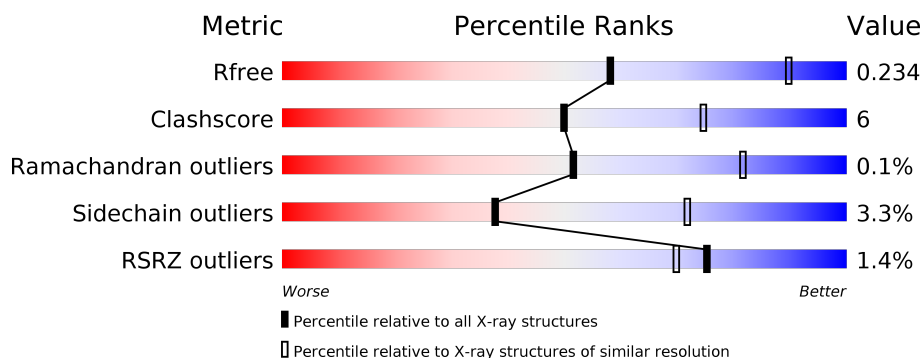
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	769	<div> <div style="width: 81%;"></div> <div style="width: 16%;"></div> <div style="width: 3%;"></div> </div> <div>81% 16% ..</div>
1	B	769	<div> <div style="width: 82%;"></div> <div style="width: 13%;"></div> <div style="width: 5%;"></div> </div> <div>82% 13% ..</div>
1	C	769	<div> <div style="width: 82%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> </div> <div>82% 15% ..</div>
1	D	769	<div> <div style="width: 83%;"></div> <div style="width: 13%;"></div> <div style="width: 4%;"></div> </div> <div>83% 13% ..</div>
1	E	769	<div> <div style="width: 3%;"></div> <div style="width: 83%;"></div> <div style="width: 10%;"></div> <div style="width: 6%;"></div> </div> <div>3% 83% 10% • 6%</div>
1	F	769	<div> <div style="width: 5%;"></div> <div style="width: 84%;"></div> <div style="width: 9%;"></div> <div style="width: 7%;"></div> </div> <div>5% 84% 9% • 7%</div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34357 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	3	0
			5933	3782	1025	1096	30			
1	B	738	Total	C	N	O	S	0	1	0
			5756	3676	995	1058	27			
1	C	755	Total	C	N	O	S	0	1	0
			5928	3784	1031	1084	29			
1	D	745	Total	C	N	O	S	0	1	0
			5795	3692	1003	1071	29			
1	E	721	Total	C	N	O	S	0	0	0
			5500	3499	957	1019	25			
1	F	718	Total	C	N	O	S	0	1	0
			5416	3443	939	1010	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1607	SER	-	expression tag	UNP Q13085
B	1607	SER	-	expression tag	UNP Q13085
C	1607	SER	-	expression tag	UNP Q13085
D	1607	SER	-	expression tag	UNP Q13085
E	1607	SER	-	expression tag	UNP Q13085
F	1607	SER	-	expression tag	UNP Q13085

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	3	Total	O	0	0
			3	3		
2	C	4	Total	O	0	0
			4	4		

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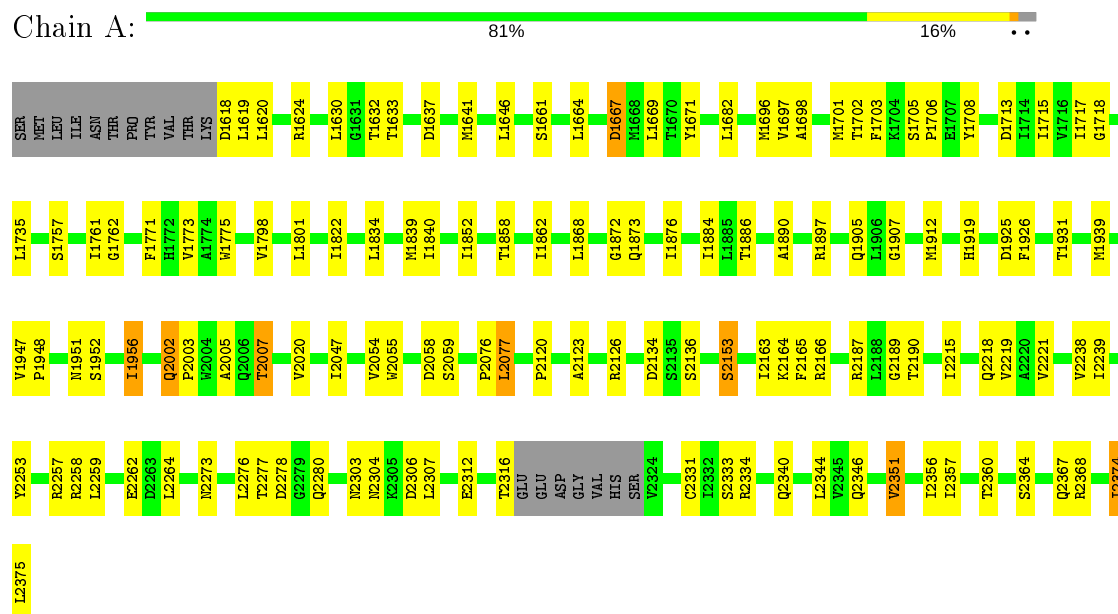
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	4	Total 4	O 4	0	0
2	E	2	Total 2	O 2	0	0
2	F	2	Total 2	O 2	0	0

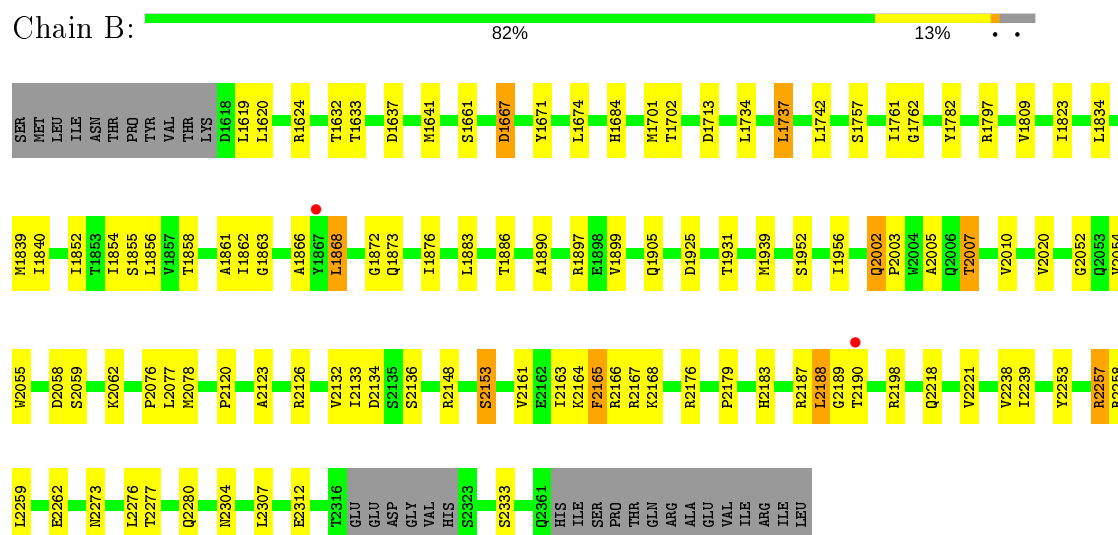
### 3 Residue-property plots [i](#)

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

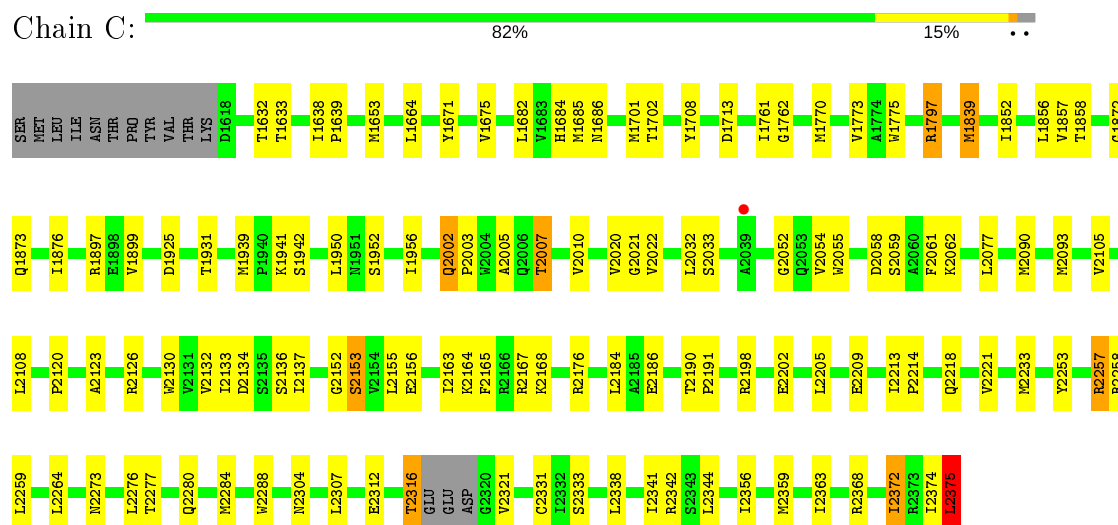
#### • Molecule 1: ACETYL-COA CARBOXYLASE 1



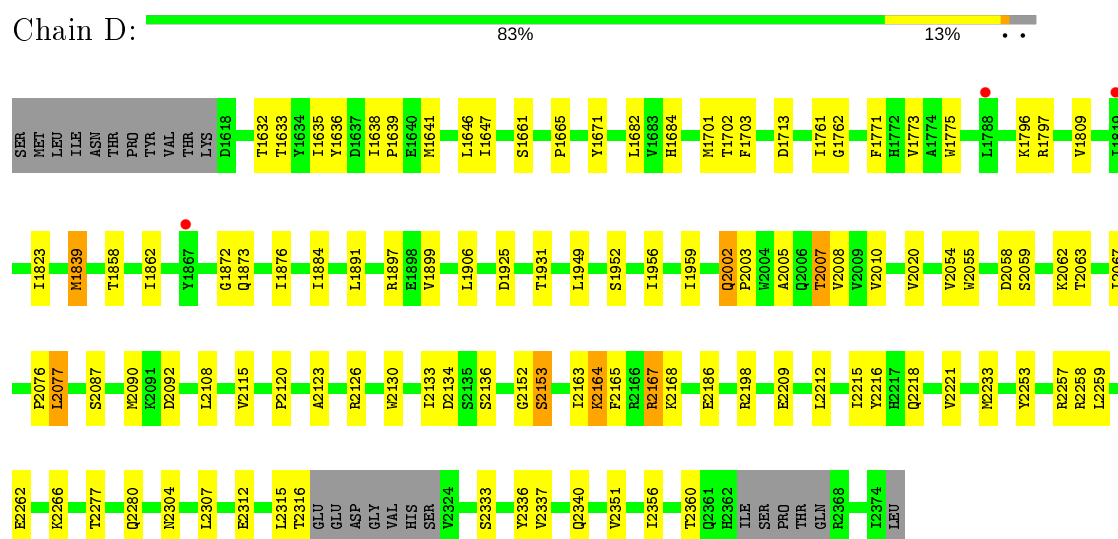
#### • Molecule 1: ACETYL-COA CARBOXYLASE 1



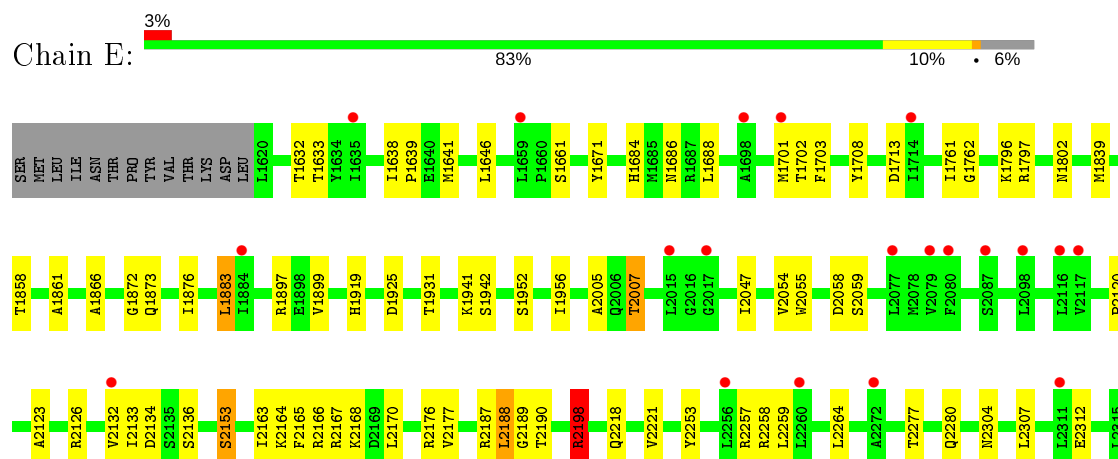
• Molecule 1: ACETYL-COA CARBOXYLASE 1

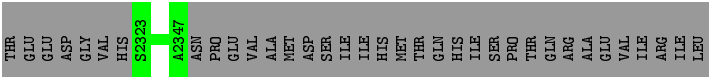


• Molecule 1: ACETYL-COA CARBOXYLASE 1

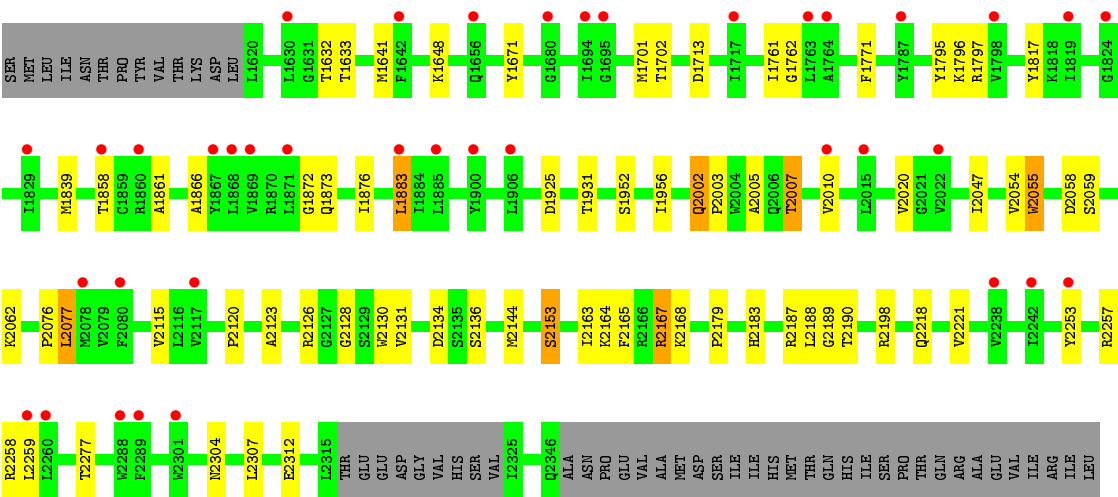
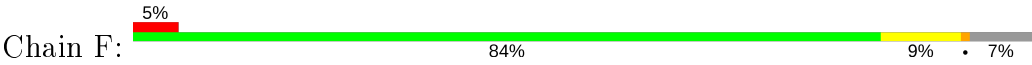


• Molecule 1: ACETYL-COA CARBOXYLASE 1





● Molecule 1: ACETYL-COA CARBOXYLASE 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.97Å 143.71Å 540.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	540.07 – 2.80 138.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (540.07-2.80) 97.9 (138.88-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.202 , 0.236 0.202 , 0.234	Depositor DCC
$R_{free}$ test set	10403 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	0.70	0/6081	0.83	3/8263 (0.0%)
1	B	0.64	0/5897	0.76	4/8021 (0.0%)
1	C	0.67	1/6071 (0.0%)	0.80	2/8254 (0.0%)
1	D	0.62	0/5933	0.76	4/8068 (0.0%)
1	E	0.55	0/5632	0.69	1/7668 (0.0%)
1	F	0.54	0/5553	0.68	3/7577 (0.0%)
All	All	0.63	1/35167 (0.0%)	0.76	17/47851 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2288	TRP	CD2-CE2	5.07	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2198	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	E	2198	ARG	CG-CD-NE	-6.39	98.38	111.80
1	A	2278	ASP	CB-CG-OD2	6.36	124.02	118.30
1	A	2077	LEU	CB-CG-CD1	-6.17	100.52	111.00
1	C	1839	MET	CG-SD-CE	6.13	110.01	100.20
1	A	1897	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	2198	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	F	2198	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	F	2198	ARG	CG-CD-NE	-5.59	100.06	111.80
1	D	1949	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	C	2375	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	1742	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	B	1734	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	B	1868	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	B	2148	ARG	CG-CD-NE	-5.03	101.24	111.80
1	D	1839	MET	CG-SD-CE	5.01	108.22	100.20
1	D	2198	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	5933	0	5799	91	0
1	B	5756	0	5562	67	0
1	C	5928	0	5775	93	0
1	D	5795	0	5575	69	0
1	E	5500	0	5152	50	0
1	F	5416	0	4973	52	0
2	A	14	0	0	1	0
2	B	3	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
All	All	34357	0	32836	388	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 6.

All (388) 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:C:2167:ARG:NH1	1:C:2209:GLU:OE2	1.75	1.18
1:A:1771:PHE:O	1:C:2176:ARG:NH1	2.04	0.90
1:E:2188:LEU:O	1:E:2198:ARG:NH2	2.08	0.86
1:A:2357:ILE:CG1	1:C:2374:ILE:HD13	2.07	0.84
1:A:1912:MET:HE3	1:C:2093:MET:CE	2.13	0.79
1:A:2357:ILE:HG13	1:C:2374:ILE:HD13	1.62	0.79
1:A:2374:ILE:O	1:A:2375:LEU:O	2.00	0.78
1:A:1912:MET:CE	1:C:2093:MET:CE	2.65	0.75
1:D:1633:THR:HG21	1:D:1641:MET:HE1	1.70	0.72
1:B:1702:THR:HG23	1:B:1713:ASP:OD1	1.90	0.72
1:C:1632:THR:OG1	1:C:1858:THR:HG21	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1632:THR:OG1	1:D:1858:THR:HG21	1.91	0.70
1:D:2007:THR:HG21	1:D:2054:VAL:O	1.91	0.70
1:E:2007:THR:HG21	1:E:2054:VAL:O	1.90	0.70
1:B:2020:VAL:HG12	1:B:2076:PRO:HG2	1.72	0.70
1:D:1665:PRO:HD2	1:E:1686:ASN:O	1.93	0.69
1:A:2020:VAL:HG12	1:A:2076:PRO:HG2	1.75	0.68
1:B:2132:VAL:HG23	1:B:2133:ILE:HG23	1.73	0.68
1:F:2130:TRP:CE2	1:F:2144:MET:HE1	2.29	0.68
1:C:2007:THR:HG21	1:C:2054:VAL:O	1.92	0.68
1:C:1675:VAL:HB	1:C:1685:MET:HE3	1.76	0.68
1:D:2315:LEU:O	1:D:2316:THR:CB	2.40	0.68
1:C:2312:GLU:O	1:C:2316:THR:HG23	1.93	0.67
1:D:1633:THR:HG21	1:D:1641:MET:CE	2.24	0.67
1:A:2007:THR:HG21	1:A:2054:VAL:O	1.94	0.67
1:D:2020:VAL:HG12	1:D:2076:PRO:HG2	1.76	0.66
1:A:1886:THR:CG2	1:A:1890:ALA:HB3	2.25	0.66
1:B:1858:THR:HG23	1:B:1925:ASP:OD1	1.95	0.66
1:A:2357:ILE:HG12	1:C:2374:ILE:HD13	1.77	0.65
1:B:2020:VAL:HG11	1:B:2078:MET:HE2	1.79	0.65
1:C:2155:LEU:HD12	1:C:2156:GLU:H	1.61	0.64
1:D:2163:ILE:HG22	1:D:2164:LYS:HG2	1.79	0.64
1:F:2007:THR:HG21	1:F:2054:VAL:O	1.96	0.64
1:C:2184:LEU:HB3	1:C:2205:LEU:HD13	1.79	0.64
1:A:2340:GLN:HA	1:A:2340:GLN:OE1	1.98	0.64
1:A:2312:GLU:O	1:A:2316:THR:HG23	1.98	0.63
1:B:1624:ARG:NH1	1:B:1637:ASP:OD1	2.31	0.63
1:F:2130:TRP:CZ2	1:F:2144:MET:HE2	2.34	0.63
1:F:1795:TYR:CD2	1:F:1817:TYR:CE2	2.87	0.63
1:E:1632:THR:OG1	1:E:1858:THR:HG21	1.98	0.62
1:C:2258:ARG:CZ	1:C:2307:LEU:HD23	2.29	0.62
1:A:1624:ARG:NH1	1:A:1637:ASP:OD1	2.33	0.62
1:F:1858:THR:HG23	1:F:1925:ASP:OD1	1.99	0.62
1:A:1858:THR:HG23	1:A:1925:ASP:OD1	2.00	0.61
1:A:2238:VAL:HG23	1:A:2239:ILE:HG23	1.80	0.61
1:C:2134:ASP:OD2	1:C:2136:SER:HB3	2.01	0.61
1:F:2128:GLY:O	1:F:2131:VAL:HG12	2.00	0.61
1:A:1702:THR:HG23	1:A:1713:ASP:OD1	2.00	0.61
1:A:2134:ASP:OD2	1:A:2136:SER:HB3	2.02	0.60
1:B:2007:THR:HG21	1:B:2054:VAL:O	2.01	0.60
1:A:2005:ALA:HB2	1:A:2058:ASP:HB2	1.84	0.59
1:C:2163:ILE:HG22	1:C:2164:LYS:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2333:SER:O	1:D:2337:VAL:HG23	2.02	0.59
1:E:1839:MET:HA	1:F:2136:SER:OG	2.01	0.59
1:C:2374:ILE:O	1:C:2375:LEU:HB3	2.02	0.59
1:E:1956:ILE:H	1:E:1956:ILE:HD12	1.67	0.59
1:A:2163:ILE:HG22	1:A:2164:LYS:HG2	1.85	0.59
1:B:1737:LEU:O	1:B:1737:LEU:HD12	2.03	0.59
1:D:2134:ASP:OD2	1:D:2136:SER:HB3	2.03	0.59
1:F:2179:PRO:O	1:F:2183[A]:HIS:ND1	2.32	0.59
1:B:2134:ASP:OD2	1:B:2136:SER:HB3	2.03	0.59
1:D:2108:LEU:HD11	1:D:2133:ILE:HG22	1.85	0.59
1:D:1897:ARG:NH1	1:D:1899:VAL:HG22	2.19	0.58
1:C:1876:ILE:HD13	1:C:1931:THR:HB	1.85	0.58
1:A:1839:MET:HA	1:C:2136:SER:OG	2.04	0.58
1:A:1912:MET:CE	1:C:2093:MET:HE2	2.33	0.58
1:C:2155:LEU:HD12	1:C:2156:GLU:N	2.19	0.57
1:F:1702:THR:HG23	1:F:1713:ASP:OD1	2.05	0.57
1:A:1905:GLN:O	1:C:2090:MET:HG3	2.03	0.57
1:B:2257:ARG:NH2	1:B:2312:GLU:OE1	2.38	0.57
1:A:2257:ARG:NH2	1:A:2312:GLU:OE1	2.37	0.57
1:A:2351:VAL:HG22	1:C:2338:LEU:HG	1.87	0.57
1:F:2005:ALA:HB2	1:F:2058:ASP:HB2	1.87	0.57
1:A:1632:THR:OG1	1:A:1858:THR:HG21	2.05	0.57
1:D:1876:ILE:HD13	1:D:1931:THR:HB	1.87	0.57
1:B:1897:ARG:NH1	1:B:1899:VAL:HG22	2.20	0.57
1:E:2134:ASP:OD2	1:E:2136:SER:HB3	2.05	0.57
1:C:2032:LEU:HD12	1:C:2033:SER:N	2.20	0.56
1:F:1795:TYR:CE2	1:F:1817:TYR:CE2	2.93	0.56
1:A:2136:SER:OG	1:C:1839:MET:HA	2.05	0.56
1:F:1956:ILE:H	1:F:1956:ILE:HD12	1.71	0.56
1:F:1632:THR:OG1	1:F:1858:THR:HG21	2.04	0.56
1:B:2179:PRO:O	1:B:2183[B]:HIS:ND1	2.39	0.56
1:E:1897:ARG:NH1	1:E:1899:VAL:HG22	2.20	0.56
1:A:1912:MET:CE	1:C:2093:MET:HE3	2.36	0.56
1:C:2276:LEU:HD22	1:C:2284:MET:HE1	1.87	0.56
1:C:2257:ARG:NH2	1:C:2312:GLU:OE1	2.39	0.56
1:F:2134:ASP:OD2	1:F:2136:SER:HB3	2.04	0.56
1:C:1956:ILE:HD12	1:C:1956:ILE:H	1.70	0.56
1:E:2005:ALA:HB2	1:E:2058:ASP:HB2	1.88	0.56
1:E:2136:SER:OG	1:F:1839:MET:HA	2.05	0.56
1:A:1912:MET:HE1	1:C:2093:MET:CE	2.35	0.55
1:B:2258:ARG:CZ	1:B:2307:LEU:HD23	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2010:VAL:HG22	1:D:2062:LYS:HE3	1.88	0.55
1:E:1858:THR:HG23	1:E:1925:ASP:OD1	2.06	0.55
1:B:1633:THR:HG21	1:B:1641:MET:HE3	1.88	0.55
1:C:2184:LEU:CB	1:C:2205:LEU:HD13	2.36	0.55
1:E:1702:THR:HG23	1:E:1713:ASP:OD1	2.07	0.55
1:E:2257:ARG:NH2	1:E:2312:GLU:OE1	2.39	0.55
1:B:2218:GLN:O	1:B:2221:VAL:HG22	2.07	0.55
1:F:2218:GLN:O	1:F:2221:VAL:HG22	2.06	0.55
1:D:1956:ILE:HD12	1:D:1956:ILE:H	1.73	0.54
1:D:2257:ARG:NH2	1:D:2312:GLU:OE1	2.40	0.54
1:B:2005:ALA:HB2	1:B:2058:ASP:HB2	1.88	0.54
1:E:1876:ILE:HD13	1:E:1931:THR:HB	1.90	0.54
1:F:2257:ARG:NH2	1:F:2312:GLU:OE1	2.41	0.54
1:E:2176:ARG:NH1	1:F:1771:PHE:O	2.38	0.54
1:C:1675:VAL:HB	1:C:1685:MET:CE	2.38	0.53
1:A:1696:MET:HB3	1:A:1735:LEU:HD23	1.89	0.53
1:B:2136:SER:OG	1:D:1839:MET:HA	2.09	0.53
1:C:1897:ARG:NH1	1:C:1899:VAL:HG22	2.24	0.53
1:A:2356:ILE:O	1:A:2360:THR:HG23	2.08	0.52
1:A:1798:VAL:HA	1:A:1801:LEU:HD12	1.92	0.52
1:B:2176:ARG:NH1	1:D:1771:PHE:O	2.39	0.52
1:F:2130:TRP:CZ2	1:F:2144:MET:CE	2.92	0.52
1:A:2356:ILE:HD11	1:C:2359:MET:HE2	1.91	0.52
1:A:2356:ILE:HG23	1:C:2356:ILE:HD13	1.90	0.52
1:D:2005:ALA:HB2	1:D:2058:ASP:HB2	1.91	0.52
1:D:2167:ARG:HB3	1:D:2167:ARG:HH11	1.75	0.52
1:B:2163:ILE:HG22	1:B:2164:LYS:HG2	1.92	0.52
1:B:1757:SER:HA	1:B:1862:ILE:HD12	1.91	0.52
1:C:2273:ASN:HB3	1:C:2276:LEU:HD12	1.92	0.51
1:F:1648:LYS:CD	1:F:1648:LYS:O	2.58	0.51
1:B:1839:MET:HA	1:D:2136:SER:OG	2.10	0.51
1:B:1632:THR:OG1	1:B:1858:THR:HG21	2.10	0.51
1:A:1761:ILE:HG22	1:A:1762:GLY:N	2.25	0.51
1:C:1708:TYR:CZ	1:C:1941:LYS:HB3	2.45	0.51
1:E:2163:ILE:HG22	1:E:2164:LYS:HG2	1.92	0.51
1:A:1717:ILE:HG22	1:A:1718:GLY:N	2.25	0.51
1:B:2238:VAL:HG23	1:B:2239:ILE:HG23	1.93	0.51
1:E:1708:TYR:CZ	1:E:1941:LYS:HB3	2.46	0.51
1:E:2218:GLN:O	1:E:2221:VAL:HG22	2.10	0.51
1:A:2356:ILE:HD13	1:C:2356:ILE:HG23	1.93	0.50
1:A:1667:ASP:OD2	1:B:1620:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2258:ARG:CZ	1:F:2307:LEU:HD23	2.42	0.50
1:A:1840:ILE:HG13	1:A:1868:LEU:HD21	1.94	0.50
1:A:2218:GLN:O	1:A:2221:VAL:HG22	2.12	0.50
1:B:1854:ILE:HG22	1:B:1855:SER:N	2.25	0.50
1:D:2163:ILE:HG22	1:D:2164:LYS:CG	2.42	0.50
1:A:1912:MET:HE1	1:C:2093:MET:HE3	1.92	0.50
1:D:2167:ARG:NE	1:D:2209:GLU:OE2	2.43	0.50
1:E:2187:ARG:O	1:E:2190:THR:HG23	2.12	0.50
1:A:1632:THR:HB	1:A:1858:THR:HG22	1.93	0.49
1:B:1862:ILE:HG22	1:B:1863:GLY:N	2.27	0.49
1:B:2010:VAL:HG22	1:B:2062:LYS:HE3	1.93	0.49
1:D:2212:LEU:O	1:D:2215:ILE:HG22	2.12	0.49
1:C:2005:ALA:HB2	1:C:2058:ASP:HB2	1.95	0.49
1:E:2187:ARG:C	1:E:2189:GLY:N	2.66	0.49
1:F:2187:ARG:C	1:F:2189:GLY:N	2.65	0.49
1:D:2120:PRO:HD2	1:D:2123:ALA:CB	2.42	0.49
1:F:2130:TRP:CE2	1:F:2144:MET:CE	2.95	0.49
1:A:1696:MET:CG	1:A:1735:LEU:HD23	2.43	0.49
1:A:2273:ASN:HB3	1:A:2276:LEU:HD12	1.95	0.49
1:D:1647:ILE:HG23	1:E:1688:LEU:HD23	1.94	0.49
1:E:1861:ALA:HB3	1:E:1883:LEU:HD13	1.94	0.49
1:B:1737:LEU:C	1:B:1737:LEU:HD12	2.33	0.49
1:E:1646:LEU:HD21	1:E:1703:PHE:HB2	1.95	0.49
1:C:2258:ARG:HG3	1:C:2259:LEU:N	2.28	0.49
1:E:2258:ARG:HD3	1:E:2304:ASN:OD1	2.13	0.49
1:A:1876:ILE:HD13	1:A:1931:THR:HB	1.95	0.48
1:A:2258:ARG:HD3	1:A:2304:ASN:OD1	2.13	0.48
1:B:1876:ILE:HD13	1:B:1931:THR:HB	1.95	0.48
1:E:2120:PRO:HD2	1:E:2123:ALA:CB	2.42	0.48
1:F:2120:PRO:HD2	1:F:2123:ALA:CB	2.43	0.48
1:A:1886:THR:HG23	1:A:1890:ALA:HB3	1.95	0.48
1:B:2120:PRO:HD2	1:B:2123:ALA:CB	2.42	0.48
1:A:2258:ARG:CZ	1:A:2307:LEU:HD23	2.43	0.48
1:B:1823:ILE:N	1:B:1823:ILE:HD13	2.29	0.48
1:D:1956:ILE:HG21	1:D:2253:TYR:CD2	2.48	0.48
1:F:1866:ALA:HA	1:F:1883:LEU:HD11	1.96	0.48
1:F:2258:ARG:HD3	1:F:2304:ASN:OD1	2.13	0.48
1:A:2187:ARG:C	1:A:2189:GLY:N	2.67	0.48
1:E:1866:ALA:HA	1:E:1883:LEU:HD11	1.95	0.48
1:F:2163:ILE:HG22	1:F:2164:LYS:HG2	1.95	0.48
1:B:1905:GLN:O	1:D:2090:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1891:LEU:HD12	1:D:1906:LEU:HD11	1.95	0.48
1:A:1646:LEU:HD21	1:A:1703:PHE:HB2	1.95	0.48
1:B:2187:ARG:C	1:B:2189:GLY:N	2.67	0.48
1:D:2063:THR:O	1:D:2067:ILE:HD12	2.14	0.48
1:F:2002:GLN:HG3	1:F:2003:PRO:HD3	1.95	0.48
1:C:2002:GLN:HG3	1:C:2003:PRO:HD3	1.95	0.48
1:E:2258:ARG:CZ	1:E:2307:LEU:HD23	2.44	0.48
1:F:2010:VAL:HG22	1:F:2062:LYS:HE3	1.96	0.48
1:A:2120:PRO:HD2	1:A:2123:ALA:CB	2.44	0.47
1:B:1632:THR:OG1	1:B:1633:THR:N	2.46	0.47
1:B:2273:ASN:HB3	1:B:2276:LEU:HD12	1.96	0.47
1:C:1632:THR:HB	1:C:1858:THR:HG22	1.94	0.47
1:E:1632:THR:OG1	1:E:1633:THR:N	2.46	0.47
1:E:1872:GLY:O	1:E:1873:GLN:HB2	2.14	0.47
1:B:2002:GLN:HG3	1:B:2003:PRO:HD3	1.96	0.47
1:D:2258:ARG:HD3	1:D:2304:ASN:OD1	2.14	0.47
1:C:1632:THR:OG1	1:C:1633:THR:N	2.47	0.47
1:C:2032:LEU:HD12	1:C:2033:SER:H	1.80	0.47
1:C:2184:LEU:HB2	1:C:2205:LEU:CD1	2.45	0.47
1:E:1956:ILE:HG21	1:E:2253:TYR:CD2	2.49	0.47
1:F:1632:THR:OG1	1:F:1633:THR:N	2.48	0.47
1:F:2007:THR:CG2	1:F:2054:VAL:O	2.63	0.47
1:B:2258:ARG:HD3	1:B:2304:ASN:OD1	2.13	0.47
1:D:2215:ILE:HG23	1:D:2216:TYR:N	2.29	0.47
1:A:1907:GLY:HA2	1:A:1912:MET:HE2	1.95	0.47
1:A:1834:LEU:HD13	1:C:2130:TRP:CD2	2.49	0.47
1:C:2276:LEU:HD22	1:C:2284:MET:CE	2.45	0.47
1:D:1632:THR:OG1	1:D:1633:THR:N	2.46	0.47
1:B:2052:GLY:O	1:B:2054:VAL:HG23	2.14	0.47
1:C:2105:VAL:HG23	1:C:2132:VAL:HG12	1.95	0.47
1:A:1630:LEU:HA	1:A:1630:LEU:HD23	1.55	0.47
1:E:1633:THR:HG21	1:E:1641:MET:HE3	1.97	0.47
1:A:2303:ASN:ND2	1:A:2306:ASP:OD2	2.48	0.47
1:B:1956:ILE:HG21	1:B:2253:TYR:CD2	2.50	0.47
1:D:1823:ILE:HD13	1:D:1823:ILE:N	2.30	0.47
1:B:1834:LEU:HD13	1:D:2130:TRP:CD2	2.50	0.47
1:F:1876:ILE:HD13	1:F:1931:THR:HB	1.97	0.47
1:F:2126:ARG:NH1	1:F:2153:SER:OG	2.48	0.47
1:B:1872:GLY:O	1:B:1873:GLN:HB2	2.14	0.47
1:D:1773:VAL:HG11	1:D:1775:TRP:CE2	2.50	0.47
1:E:2132:VAL:HG23	1:E:2133:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1761:ILE:HG22	1:F:1762:GLY:N	2.29	0.47
1:B:1840:ILE:HG13	1:B:1868:LEU:HD21	1.97	0.46
1:C:1872:GLY:O	1:C:1873:GLN:HB2	2.15	0.46
1:B:2161:VAL:HG13	1:B:2165:PHE:HB3	1.96	0.46
1:D:1632:THR:HB	1:D:1858:THR:HG22	1.96	0.46
1:F:1872:GLY:O	1:F:1873:GLN:HB2	2.15	0.46
1:A:1761:ILE:CG2	1:A:1762:GLY:N	2.78	0.46
1:D:1872:GLY:O	1:D:1873:GLN:HB2	2.15	0.46
1:D:2258:ARG:CZ	1:D:2307:LEU:HD23	2.46	0.46
1:A:2126:ARG:NH1	1:A:2153:SER:OG	2.49	0.46
1:C:1653:MET:CE	1:C:1950:LEU:HD11	2.45	0.46
1:C:2120:PRO:HD2	1:C:2123:ALA:CB	2.46	0.46
1:B:1886:THR:CG2	1:B:1890:ALA:HB3	2.46	0.46
1:C:1773:VAL:HG11	1:C:1775:TRP:CE2	2.51	0.46
1:D:2218:GLN:O	1:D:2221:VAL:HG22	2.16	0.46
1:C:2213:ILE:HG22	1:C:2214:PRO:N	2.30	0.46
1:A:2258:ARG:HG3	1:A:2259:LEU:N	2.31	0.46
1:A:2344:LEU:HD12	1:C:2341:ILE:HG13	1.98	0.46
1:B:1671:TYR:HB3	1:B:1701:MET:HG2	1.98	0.46
1:B:1956:ILE:H	1:B:1956:ILE:HD12	1.80	0.46
1:B:2126:ARG:NH1	1:B:2153:SER:OG	2.49	0.46
1:A:1632:THR:OG1	1:A:1633:THR:N	2.47	0.46
1:E:2126:ARG:NH1	1:E:2153:SER:OG	2.48	0.46
1:D:1702:THR:HG23	1:D:1713:ASP:OD1	2.16	0.45
1:A:1633:THR:HG21	1:A:1641:MET:HE3	1.98	0.45
1:B:2163:ILE:O	1:B:2166:ARG:NH1	2.47	0.45
1:C:2134:ASP:O	1:C:2137:ILE:HD12	2.16	0.45
1:A:1696:MET:CB	1:A:1735:LEU:HD23	2.45	0.45
1:B:2007:THR:HB	2:B:3001:HOH:O	2.16	0.45
1:C:1761:ILE:HG22	1:C:1762:GLY:N	2.31	0.45
1:C:2273:ASN:HB3	1:C:2276:LEU:CD1	2.47	0.45
1:A:1852:ILE:HD13	1:A:1939:MET:SD	2.57	0.45
1:C:1858:THR:HG23	1:C:1925:ASP:OD1	2.15	0.45
1:D:2126:ARG:NH1	1:D:2153:SER:OG	2.50	0.45
1:F:2259:LEU:HA	1:F:2259:LEU:HD23	1.75	0.45
1:B:2258:ARG:HG3	1:B:2259:LEU:N	2.31	0.45
1:C:2198:ARG:NE	1:C:2202:GLU:OE2	2.46	0.45
1:A:1757:SER:HA	1:A:1862:ILE:HD12	1.98	0.45
1:C:2258:ARG:HD3	1:C:2304:ASN:OD1	2.17	0.45
1:C:2338:LEU:HD23	1:C:2338:LEU:HA	1.74	0.45
1:A:1839:MET:CA	1:C:2136:SER:OG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1956:ILE:HD12	1:C:1956:ILE:N	2.32	0.45
1:E:2163:ILE:O	1:E:2166:ARG:NH1	2.46	0.45
1:D:2002:GLN:HG3	1:D:2003:PRO:HD3	1.99	0.45
1:D:2008:VAL:HG13	1:D:2062:LYS:HE2	1.98	0.45
1:B:1674:LEU:HD21	1:B:1684:HIS:CE1	2.51	0.45
1:C:2126:ARG:NH1	1:C:2153:SER:OG	2.50	0.45
1:E:2187:ARG:O	1:E:2190:THR:N	2.49	0.45
1:A:1669:LEU:HD12	1:A:1703:PHE:HB3	1.99	0.44
1:C:2108:LEU:HD11	1:C:2133:ILE:HG22	1.99	0.44
1:F:1956:ILE:HG21	1:F:2253:TYR:CD2	2.52	0.44
1:B:1854:ILE:CG2	1:B:1855:SER:N	2.80	0.44
1:D:2356:ILE:O	1:D:2360:THR:HG23	2.17	0.44
1:B:1852:ILE:HD13	1:B:1939:MET:SD	2.57	0.44
1:C:1770:MET:HE1	1:C:1797:ARG:HH21	1.82	0.44
1:C:1941:LYS:HG2	1:C:1942:SER:N	2.33	0.44
1:C:1671:TYR:HB3	1:C:1701:MET:HG2	2.00	0.44
1:C:2052:GLY:O	1:C:2054:VAL:HG23	2.18	0.44
1:A:1872:GLY:O	1:A:1873:GLN:HB2	2.17	0.44
1:C:1702:THR:HG23	1:C:1713:ASP:OD1	2.17	0.44
1:F:1633:THR:HG21	1:F:1641:MET:HE3	1.99	0.44
1:E:1956:ILE:N	1:E:1956:ILE:HD12	2.31	0.44
1:A:1671:TYR:HB3	1:A:1701:MET:HG2	1.99	0.44
1:A:1956:ILE:HG21	1:A:2253:TYR:CD2	2.52	0.44
1:C:1770:MET:HE1	1:C:1797:ARG:NH2	2.32	0.44
1:C:2020:VAL:HG23	1:C:2022:VAL:CG2	2.48	0.44
1:F:1956:ILE:HD12	1:F:1956:ILE:N	2.33	0.44
1:E:2167:ARG:O	1:E:2168:LYS:C	2.56	0.44
1:E:2258:ARG:HG3	1:E:2259:LEU:N	2.32	0.44
1:D:2007:THR:HB	1:D:2059:SER:OG	2.18	0.43
1:D:2258:ARG:HG3	1:D:2259:LEU:N	2.32	0.43
1:D:2152:GLY:HA3	1:D:2233:MET:CE	2.48	0.43
1:A:1705:SER:HB2	1:A:1706:PRO:HD2	1.99	0.43
1:E:2167:ARG:HA	1:E:2170:LEU:HD12	2.00	0.43
1:D:1682:LEU:HA	1:D:1682:LEU:HD12	1.79	0.43
1:A:2058:ASP:OD1	1:A:2059:SER:N	2.51	0.43
1:D:1633:THR:CG2	1:D:1641:MET:HE1	2.45	0.43
1:F:2187:ARG:O	1:F:2189:GLY:N	2.52	0.43
1:C:2372:ILE:O	1:C:2375:LEU:HD22	2.19	0.43
1:E:1761:ILE:HG22	1:E:1762:GLY:N	2.32	0.43
1:D:1671:TYR:HB3	1:D:1701:MET:HG2	2.01	0.43
1:D:2007:THR:CG2	1:D:2054:VAL:O	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1632:THR:HB	1:E:1858:THR:HG22	2.00	0.43
1:F:2258:ARG:HG3	1:F:2259:LEU:N	2.33	0.43
1:A:2364:SER:O	1:A:2367:GLN:N	2.50	0.43
1:C:1856:LEU:HD12	1:C:1857:VAL:N	2.33	0.43
1:C:2021:GLY:C	1:C:2022:VAL:HG23	2.39	0.43
1:A:2258:ARG:NH2	1:A:2262:GLU:OE1	2.49	0.43
1:D:1646:LEU:HD21	1:D:1703:PHE:HB2	2.00	0.43
1:D:1858:THR:HG23	1:D:1925:ASP:OD1	2.19	0.43
1:F:2020:VAL:HG12	1:F:2076:PRO:HG2	2.00	0.43
1:B:2007:THR:HB	1:B:2059:SER:OG	2.19	0.42
1:C:2163:ILE:HG22	1:C:2164:LYS:CG	2.48	0.42
1:A:2007:THR:CG2	1:A:2007:THR:O	2.66	0.42
1:C:1638:ILE:HB	1:C:1639:PRO:HD3	2.01	0.42
1:E:1839:MET:CA	1:F:2136:SER:OG	2.67	0.42
1:F:2167:ARG:O	1:F:2168:LYS:C	2.57	0.42
1:F:1671:TYR:HB3	1:F:1701:MET:HG2	2.00	0.42
1:A:2007:THR:HB	2:A:3012:HOH:O	2.20	0.42
1:B:1761:ILE:HG22	1:B:1762:GLY:N	2.35	0.42
1:B:2258:ARG:NH2	1:B:2262:GLU:OE1	2.47	0.42
1:C:2258:ARG:CZ	1:C:2307:LEU:CD2	2.97	0.42
1:A:1682:LEU:HD12	1:A:1682:LEU:HA	1.89	0.42
1:C:2276:LEU:CD2	1:C:2284:MET:HE1	2.48	0.42
1:D:1773:VAL:HG11	1:D:1775:TRP:CZ2	2.55	0.42
1:D:2262:GLU:HG2	1:D:2266:LYS:HE2	2.02	0.42
1:B:2188:LEU:O	1:B:2198:ARG:NH2	2.53	0.42
1:D:1635:ILE:HG23	1:D:1636:TYR:N	2.34	0.42
1:A:2187:ARG:O	1:A:2190:THR:N	2.51	0.42
1:B:2058:ASP:OD1	1:B:2059:SER:N	2.53	0.42
1:D:1761:ILE:HG22	1:D:1762:GLY:N	2.35	0.42
1:A:2215:ILE:O	1:A:2219:VAL:HG23	2.19	0.41
1:B:2187:ARG:O	1:B:2190:THR:N	2.51	0.41
1:C:2010:VAL:HG22	1:C:2062:LYS:HE3	2.02	0.41
1:C:1956:ILE:HG21	1:C:2253:TYR:CD2	2.55	0.41
1:E:2007:THR:HB	1:E:2059:SER:OG	2.19	0.41
1:B:1862:ILE:CG2	1:B:1863:GLY:N	2.81	0.41
1:E:1638:ILE:HB	1:E:1639:PRO:HD3	2.02	0.41
1:F:2058:ASP:OD1	1:F:2059:SER:N	2.54	0.41
1:A:1620:LEU:HA	1:A:1620:LEU:HD12	1.83	0.41
1:A:1926:PHE:C	1:A:1926:PHE:CD1	2.94	0.41
1:A:1956:ILE:HD12	1:A:1956:ILE:H	1.86	0.41
1:A:2007:THR:HB	1:A:2059:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1852:ILE:HD13	1:C:1939:MET:SD	2.61	0.41
1:D:1761:ILE:HD13	1:D:1761:ILE:HG21	1.87	0.41
1:A:2163:ILE:O	1:A:2166:ARG:NH1	2.47	0.41
1:A:2187:ARG:O	1:A:2189:GLY:N	2.53	0.41
1:C:2184:LEU:CB	1:C:2205:LEU:CD1	2.99	0.41
1:D:1638:ILE:HB	1:D:1639:PRO:HD3	2.02	0.41
1:E:2187:ARG:O	1:E:2189:GLY:N	2.54	0.41
1:A:1697:VAL:HG12	1:A:1698:ALA:N	2.36	0.41
1:B:1866:ALA:HA	1:B:1883:LEU:HD11	2.02	0.41
1:B:2187:ARG:O	1:B:2189:GLY:N	2.53	0.41
1:D:2167:ARG:O	1:D:2168:LYS:C	2.59	0.41
1:D:1862:ILE:CD1	1:D:1884:ILE:HG12	2.51	0.41
1:E:1671:TYR:HB3	1:E:1701:MET:HG2	2.02	0.41
1:A:1624:ARG:NH2	1:B:1667:ASP:OD2	2.53	0.41
1:B:1856:LEU:HD13	1:B:1876:ILE:HB	2.03	0.41
1:C:2007:THR:HB	1:C:2059:SER:OG	2.21	0.41
1:C:2152:GLY:HA3	1:C:2233:MET:CE	2.50	0.41
1:D:1862:ILE:HD13	1:D:1884:ILE:HG12	2.01	0.41
1:D:2336:TYR:CE2	1:D:2340:GLN:OE1	2.73	0.41
1:E:2007:THR:CG2	1:E:2054:VAL:O	2.65	0.41
1:F:2179:PRO:C	1:F:2183[A]:HIS:HD1	2.21	0.41
1:B:2167:ARG:O	1:B:2168:LYS:C	2.58	0.41
1:F:2007:THR:HB	1:F:2059:SER:OG	2.20	0.41
1:A:1773:VAL:HG11	1:A:1775:TRP:CE2	2.55	0.41
1:B:1861:ALA:HB3	1:B:1883:LEU:HD13	2.02	0.41
1:F:2054:VAL:HG12	1:F:2055:TRP:N	2.36	0.41
1:A:1708:TYR:CE2	1:A:1948:PRO:HB3	2.56	0.41
1:C:2007:THR:CG2	1:C:2054:VAL:O	2.66	0.41
1:C:1682:LEU:HD12	1:C:1682:LEU:HA	1.85	0.40
1:C:2167:ARG:O	1:C:2168:LYS:C	2.60	0.40
1:C:2321:VAL:O	1:C:2321:VAL:HG22	2.21	0.40
1:C:2218:GLN:O	1:C:2221:VAL:HG22	2.21	0.40
1:A:1715:ILE:HD13	1:A:1715:ILE:HA	1.86	0.40
1:A:2002:GLN:N	1:A:2003:PRO:CD	2.85	0.40
1:D:2002:GLN:N	1:D:2003:PRO:CD	2.84	0.40
1:F:1861:ALA:HB3	1:F:1883:LEU:HD13	2.03	0.40
1:F:2187:ARG:O	1:F:2190:THR:N	2.54	0.40
1:A:1822:ILE:HG21	1:A:1822:ILE:HD13	1.87	0.40
1:C:2190:THR:HA	1:C:2191:PRO:HD3	1.96	0.40
1:D:2058:ASP:OD1	1:D:2059:SER:N	2.54	0.40
1:D:2077:LEU:HB2	1:D:2115:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1941:LYS:HG2	1:E:1942:SER:N	2.35	0.40
1:A:1884:ILE:HG22	1:A:1907:GLY:HA3	2.04	0.40
1:B:1782:TYR:CZ	1:D:2215:ILE:HB	2.56	0.40
1:C:1675:VAL:CB	1:C:1685:MET:HE3	2.48	0.40
1:D:2087:SER:HG	1:D:2092:ASP:CG	2.24	0.40
1:E:2058:ASP:OD1	1:E:2059:SER:N	2.54	0.40
1:E:2187:ARG:HA	1:E:2190:THR:HG23	2.03	0.40
1:F:2077:LEU:HB2	1:F:2115:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	750/769 (98%)	716 (96%)	34 (4%)	0	100	100
1	B	735/769 (96%)	710 (97%)	24 (3%)	1 (0%)	51	81
1	C	752/769 (98%)	722 (96%)	30 (4%)	0	100	100
1	D	740/769 (96%)	712 (96%)	27 (4%)	1 (0%)	51	81
1	E	717/769 (93%)	692 (96%)	23 (3%)	2 (0%)	41	72
1	F	715/769 (93%)	688 (96%)	25 (4%)	2 (0%)	41	72
All	All	4409/4614 (96%)	4240 (96%)	163 (4%)	6 (0%)	51	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2188	LEU
1	E	1796	LYS
1	E	2188	LEU
1	F	2188	LEU

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Mol	Chain	Res	Type
1	D	1796	LYS
1	F	1796	LYS

### 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	630/672 (94%)	603 (96%)	27 (4%)	29	62
1	B	597/672 (89%)	580 (97%)	17 (3%)	43	77
1	C	620/672 (92%)	594 (96%)	26 (4%)	30	63
1	D	599/672 (89%)	581 (97%)	18 (3%)	41	75
1	E	545/672 (81%)	528 (97%)	17 (3%)	40	74
1	F	525/672 (78%)	513 (98%)	12 (2%)	50	82
All	All	3516/4032 (87%)	3399 (97%)	117 (3%)	38	72

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1618	ASP
1	A	1619	LEU
1	A	1661	SER
1	A	1664	LEU
1	A	1667	ASP
1	A	1919	HIS
1	A	1947	VAL
1	A	1951	ASN
1	A	1952	SER
1	A	1956	ILE
1	A	2002	GLN
1	A	2007	THR
1	A	2047	ILE
1	A	2055	TRP
1	A	2077	LEU
1	A	2153	SER

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Mol	Chain	Res	Type
1	A	2165	PHE
1	A	2264	LEU
1	A	2277	THR
1	A	2280	GLN
1	A	2331	CYS
1	A	2333	SER
1	A	2334	ARG
1	A	2346	GLN
1	A	2351	VAL
1	A	2368	ARG
1	A	2374	ILE
1	B	1619	LEU
1	B	1661	SER
1	B	1667	ASP
1	B	1737	LEU
1	B	1797	ARG
1	B	1809	VAL
1	B	1952	SER
1	B	2002	GLN
1	B	2007	THR
1	B	2055	TRP
1	B	2077	LEU
1	B	2153	SER
1	B	2165	PHE
1	B	2257	ARG
1	B	2277	THR
1	B	2280	GLN
1	B	2333	SER
1	C	1664	LEU
1	C	1684	HIS
1	C	1686	ASN
1	C	1797	ARG
1	C	1952	SER
1	C	2002	GLN
1	C	2007	THR
1	C	2055	TRP
1	C	2061	PHE
1	C	2077	LEU
1	C	2153	SER
1	C	2165	PHE
1	C	2186	GLU
1	C	2257	ARG

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Mol	Chain	Res	Type
1	C	2264	LEU
1	C	2277	THR
1	C	2280	GLN
1	C	2316	THR
1	C	2331	CYS
1	C	2333	SER
1	C	2342	ARG
1	C	2344	LEU
1	C	2363	ILE
1	C	2368	ARG
1	C	2372	ILE
1	C	2375	LEU
1	D	1661	SER
1	D	1684	HIS
1	D	1797	ARG
1	D	1809	VAL
1	D	1952	SER
1	D	1959	ILE
1	D	2002	GLN
1	D	2007	THR
1	D	2055	TRP
1	D	2077	LEU
1	D	2153	SER
1	D	2164	LYS
1	D	2165	PHE
1	D	2167	ARG
1	D	2186	GLU
1	D	2277	THR
1	D	2280	GLN
1	D	2351	VAL
1	E	1661	SER
1	E	1684	HIS
1	E	1797	ARG
1	E	1802	ASN
1	E	1883	LEU
1	E	1919	HIS
1	E	1952	SER
1	E	2007	THR
1	E	2047	ILE
1	E	2055	TRP
1	E	2153	SER
1	E	2165	PHE

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Mol	Chain	Res	Type
1	E	2177	VAL
1	E	2198	ARG
1	E	2264	LEU
1	E	2277	THR
1	E	2280	GLN
1	F	1797	ARG
1	F	1883	LEU
1	F	1952	SER
1	F	2002	GLN
1	F	2007	THR
1	F	2047	ILE
1	F	2055	TRP
1	F	2077	LEU
1	F	2153	SER
1	F	2165	PHE
1	F	2167	ARG
1	F	2277	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2071	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	751/769 (97%)	0.06	0 <span>100</span> <span>100</span>	30, 58, 100, 148	0
1	B	738/769 (95%)	0.02	2 (0%) <span>94</span> <span>93</span>	35, 72, 123, 161	0
1	C	755/769 (98%)	0.05	1 (0%) <span>95</span> <span>95</span>	30, 69, 111, 164	0
1	D	745/769 (96%)	0.08	3 (0%) <span>92</span> <span>91</span>	41, 71, 135, 192	0
1	E	721/769 (93%)	0.21	20 (2%) 53 43	63, 101, 187, 240	0
1	F	718/769 (93%)	0.34	38 (5%) 26 17	67, 112, 176, 202	0
All	All	4428/4614 (95%)	0.13	64 (1%) <span>75</span> <span>70</span>	30, 81, 150, 240	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2238	VAL	4.0
1	F	2015	LEU	3.7
1	F	1764	ALA	3.7
1	F	1867	TYR	3.7
1	F	1763	LEU	3.3
1	F	1824	GLY	3.1
1	F	1630	LEU	3.0
1	F	2022	VAL	2.9
1	D	1819	ILE	2.9
1	F	1868	LEU	2.9
1	F	1858	THR	2.9
1	F	1871	LEU	2.8
1	F	2080	PHE	2.8
1	F	2301	TRP	2.8
1	E	2117	VAL	2.8
1	E	1701	MET	2.8
1	F	1656	GLN	2.8
1	E	2116	LEU	2.8
1	F	1680	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	1717	ILE	2.7
1	F	1829	ILE	2.7
1	C	2039	ALA	2.7
1	F	2260	LEU	2.7
1	F	1819	ILE	2.6
1	E	2079	VAL	2.6
1	F	1798	VAL	2.6
1	E	2087	SER	2.6
1	F	1642	PHE	2.6
1	E	2256	LEU	2.5
1	B	2190	THR	2.5
1	F	1869	VAL	2.5
1	F	2253	TYR	2.5
1	E	2272	ALA	2.5
1	F	1885	LEU	2.4
1	E	2077	LEU	2.4
1	F	2078	MET	2.4
1	E	1659	LEU	2.4
1	E	1714	ILE	2.3
1	E	2260	LEU	2.3
1	B	1867	TYR	2.3
1	E	2311	LEU	2.3
1	F	1860	ARG	2.2
1	F	2288	TRP	2.2
1	F	2289	PHE	2.2
1	F	1883	LEU	2.2
1	E	2015	LEU	2.2
1	F	2010	VAL	2.2
1	D	1788	LEU	2.2
1	F	2259	LEU	2.2
1	F	1694	ILE	2.1
1	E	1698	ALA	2.1
1	E	2132	VAL	2.1
1	E	1635	ILE	2.1
1	E	1884	ILE	2.1
1	F	2242	ILE	2.1
1	D	1867	TYR	2.1
1	E	2017	GLY	2.1
1	F	1695	GLY	2.1
1	F	1787	TYR	2.1
1	F	2117	VAL	2.0
1	E	2098	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	1900	TYR	2.0
1	E	2080	PHE	2.0
1	F	1906	LEU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.