



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:56 pm BST

PDB ID : 2QFY  
Title : Crystal structure of *Saccharomyces cerevesiae* mitochondrial NADP(+)-dependent isocitrate dehydrogenase in complex with  $\alpha$ -ketoglutarate  
Authors : Peng, Y.J.; Ding, J.P.  
Deposited on : 2007-06-28  
Resolution : 2.10 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

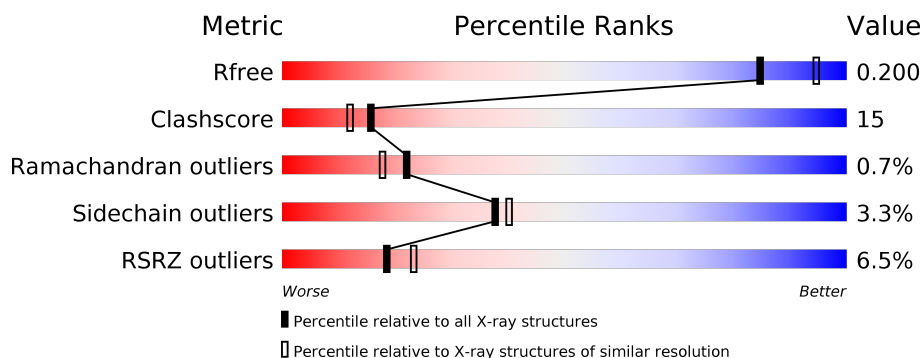
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	427	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	427	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	427	<div> <div>9%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div>
1	D	427	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• •</div> </div> </div>
1	E	427	<div> <div>11%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	F	427	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>• •</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AKG	B	2002	-	-	-	X
2	AKG	C	2003	-	-	-	X
2	AKG	D	2004	-	-	-	X
2	AKG	E	2005	-	-	-	X
2	AKG	F	2006	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20960 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 Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3256	2076	551	617	12			
1	B	411	Total	C	N	O	S	0	0	0
			3253	2073	551	617	12			
1	C	411	Total	C	N	O	S	0	0	0
			3253	2073	551	617	12			
1	D	411	Total	C	N	O	S	0	0	0
			3256	2076	551	617	12			
1	E	411	Total	C	N	O	S	0	0	0
			3253	2073	551	617	12			
1	F	411	Total	C	N	O	S	0	0	0
			3256	2076	551	617	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P21954
A	-12	HIS	-	EXPRESSION TAG	UNP P21954
A	-11	HIS	-	EXPRESSION TAG	UNP P21954
A	-10	HIS	-	EXPRESSION TAG	UNP P21954
A	-9	HIS	-	EXPRESSION TAG	UNP P21954
A	-8	HIS	-	EXPRESSION TAG	UNP P21954
A	-7	HIS	-	EXPRESSION TAG	UNP P21954
A	-6	ALA	-	EXPRESSION TAG	UNP P21954
A	-5	MET	-	EXPRESSION TAG	UNP P21954
A	-4	GLY	-	EXPRESSION TAG	UNP P21954
A	-3	ILE	-	EXPRESSION TAG	UNP P21954
A	-2	PRO	-	EXPRESSION TAG	UNP P21954
A	-1	GLY	-	EXPRESSION TAG	UNP P21954
A	0	HIS	-	EXPRESSION TAG	UNP P21954
B	-13	MET	-	EXPRESSION TAG	UNP P21954
B	-12	HIS	-	EXPRESSION TAG	UNP P21954
B	-11	HIS	-	EXPRESSION TAG	UNP P21954

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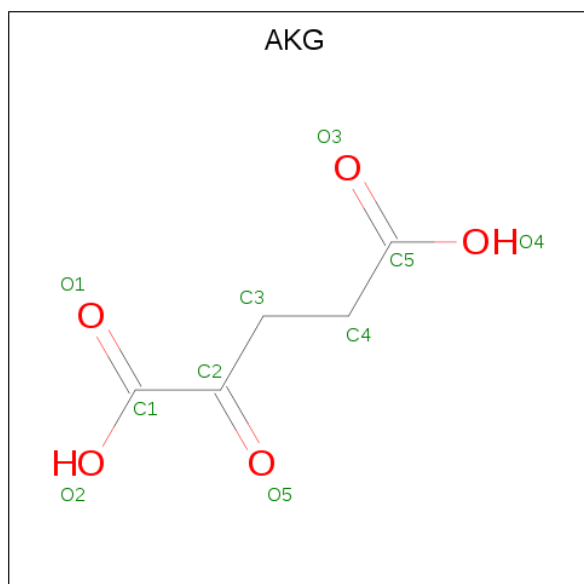
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP P21954
B	-9	HIS	-	EXPRESSION TAG	UNP P21954
B	-8	HIS	-	EXPRESSION TAG	UNP P21954
B	-7	HIS	-	EXPRESSION TAG	UNP P21954
B	-6	ALA	-	EXPRESSION TAG	UNP P21954
B	-5	MET	-	EXPRESSION TAG	UNP P21954
B	-4	GLY	-	EXPRESSION TAG	UNP P21954
B	-3	ILE	-	EXPRESSION TAG	UNP P21954
B	-2	PRO	-	EXPRESSION TAG	UNP P21954
B	-1	GLY	-	EXPRESSION TAG	UNP P21954
B	0	HIS	-	EXPRESSION TAG	UNP P21954
C	-13	MET	-	EXPRESSION TAG	UNP P21954
C	-12	HIS	-	EXPRESSION TAG	UNP P21954
C	-11	HIS	-	EXPRESSION TAG	UNP P21954
C	-10	HIS	-	EXPRESSION TAG	UNP P21954
C	-9	HIS	-	EXPRESSION TAG	UNP P21954
C	-8	HIS	-	EXPRESSION TAG	UNP P21954
C	-7	HIS	-	EXPRESSION TAG	UNP P21954
C	-6	ALA	-	EXPRESSION TAG	UNP P21954
C	-5	MET	-	EXPRESSION TAG	UNP P21954
C	-4	GLY	-	EXPRESSION TAG	UNP P21954
C	-3	ILE	-	EXPRESSION TAG	UNP P21954
C	-2	PRO	-	EXPRESSION TAG	UNP P21954
C	-1	GLY	-	EXPRESSION TAG	UNP P21954
C	0	HIS	-	EXPRESSION TAG	UNP P21954
D	-13	MET	-	EXPRESSION TAG	UNP P21954
D	-12	HIS	-	EXPRESSION TAG	UNP P21954
D	-11	HIS	-	EXPRESSION TAG	UNP P21954
D	-10	HIS	-	EXPRESSION TAG	UNP P21954
D	-9	HIS	-	EXPRESSION TAG	UNP P21954
D	-8	HIS	-	EXPRESSION TAG	UNP P21954
D	-7	HIS	-	EXPRESSION TAG	UNP P21954
D	-6	ALA	-	EXPRESSION TAG	UNP P21954
D	-5	MET	-	EXPRESSION TAG	UNP P21954
D	-4	GLY	-	EXPRESSION TAG	UNP P21954
D	-3	ILE	-	EXPRESSION TAG	UNP P21954
D	-2	PRO	-	EXPRESSION TAG	UNP P21954
D	-1	GLY	-	EXPRESSION TAG	UNP P21954
D	0	HIS	-	EXPRESSION TAG	UNP P21954
E	-13	MET	-	EXPRESSION TAG	UNP P21954
E	-12	HIS	-	EXPRESSION TAG	UNP P21954
E	-11	HIS	-	EXPRESSION TAG	UNP P21954

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP P21954
E	-9	HIS	-	EXPRESSION TAG	UNP P21954
E	-8	HIS	-	EXPRESSION TAG	UNP P21954
E	-7	HIS	-	EXPRESSION TAG	UNP P21954
E	-6	ALA	-	EXPRESSION TAG	UNP P21954
E	-5	MET	-	EXPRESSION TAG	UNP P21954
E	-4	GLY	-	EXPRESSION TAG	UNP P21954
E	-3	ILE	-	EXPRESSION TAG	UNP P21954
E	-2	PRO	-	EXPRESSION TAG	UNP P21954
E	-1	GLY	-	EXPRESSION TAG	UNP P21954
E	0	HIS	-	EXPRESSION TAG	UNP P21954
F	-13	MET	-	EXPRESSION TAG	UNP P21954
F	-12	HIS	-	EXPRESSION TAG	UNP P21954
F	-11	HIS	-	EXPRESSION TAG	UNP P21954
F	-10	HIS	-	EXPRESSION TAG	UNP P21954
F	-9	HIS	-	EXPRESSION TAG	UNP P21954
F	-8	HIS	-	EXPRESSION TAG	UNP P21954
F	-7	HIS	-	EXPRESSION TAG	UNP P21954
F	-6	ALA	-	EXPRESSION TAG	UNP P21954
F	-5	MET	-	EXPRESSION TAG	UNP P21954
F	-4	GLY	-	EXPRESSION TAG	UNP P21954
F	-3	ILE	-	EXPRESSION TAG	UNP P21954
F	-2	PRO	-	EXPRESSION TAG	UNP P21954
F	-1	GLY	-	EXPRESSION TAG	UNP P21954
F	0	HIS	-	EXPRESSION TAG	UNP P21954

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



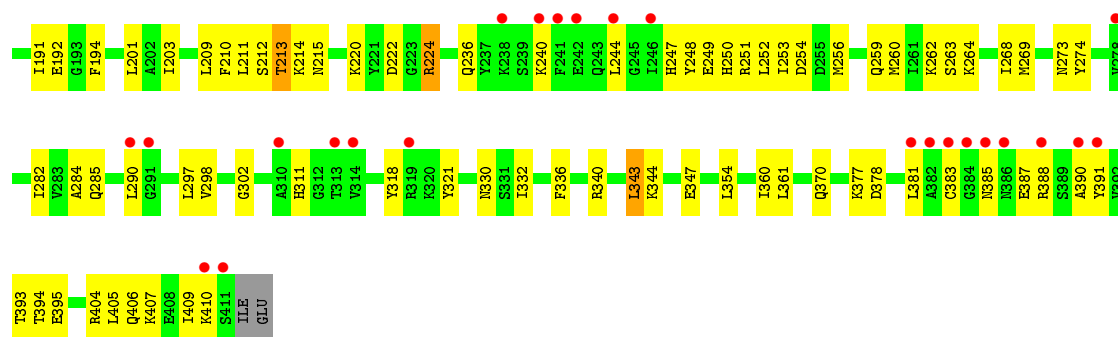
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 10 5 5	0	0
2	E	1	Total C O 10 5 5	0	0
2	F	1	Total C O 10 5 5	0	0

- Molecule 3 is water.

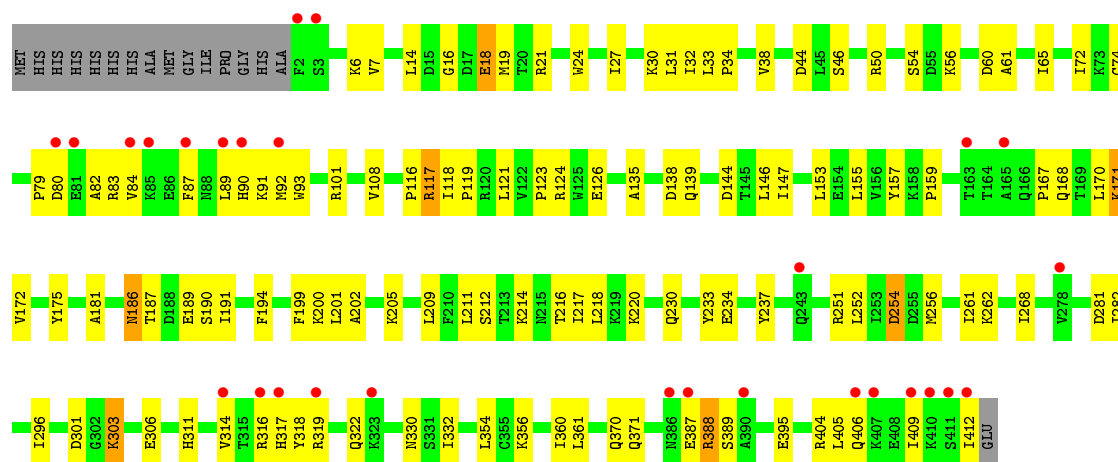
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	392	Total O 392 392	0	0
3	B	328	Total O 328 328	0	0
3	C	167	Total O 167 167	0	0
3	D	151	Total O 151 151	0	0
3	E	130	Total O 130 130	0	0
3	F	205	Total O 205 205	0	0



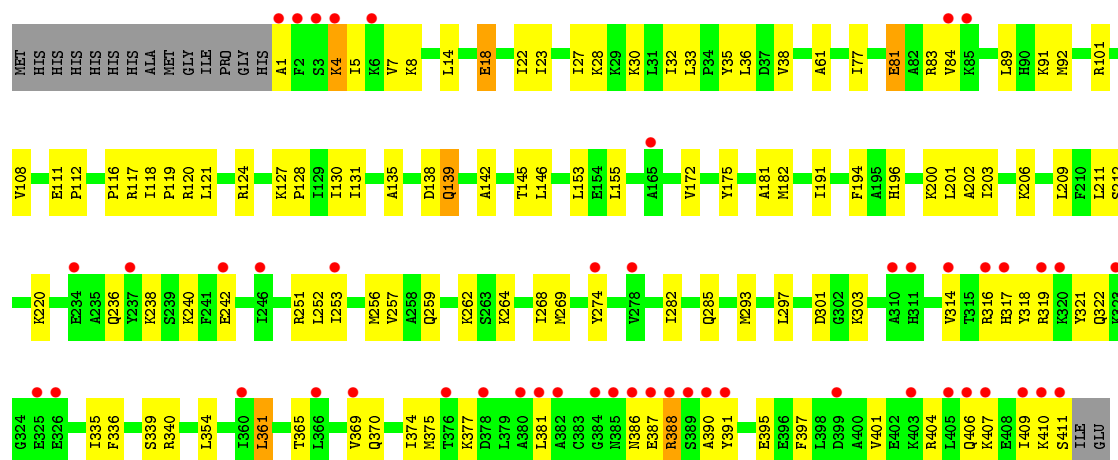




• Molecule 1: Isocitrate dehydrogenase [NADP]

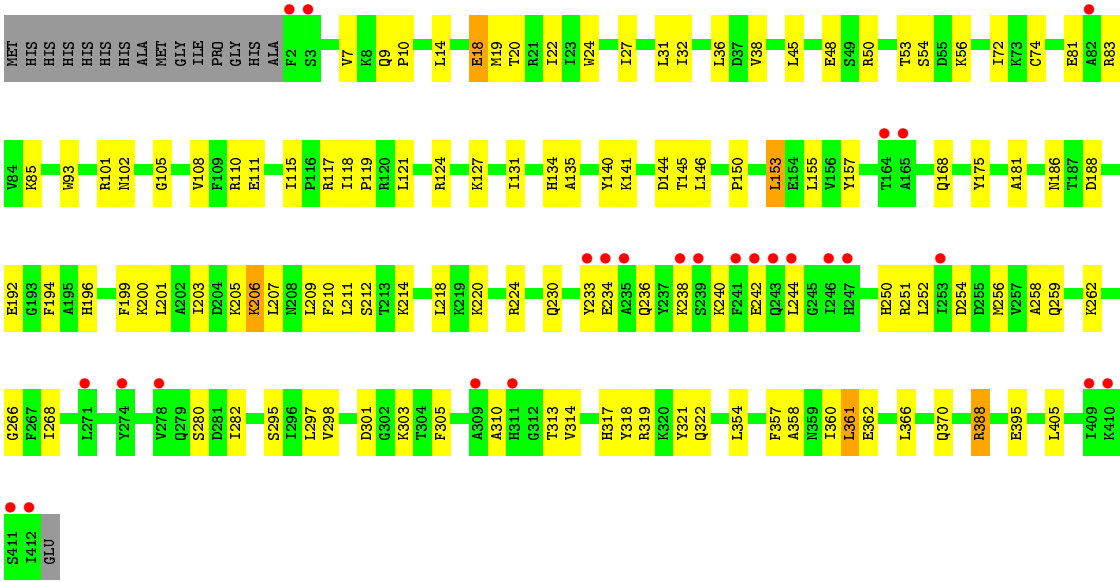


• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.90 Å 98.48 Å 190.60 Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	43.65 – 2.10 43.65 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.65-2.10) 98.3 (43.65-2.08)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.08 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.247 0.203 , 0.200	Depositor DCC
$R_{free}$ test set	8055 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.36	0/3319	0.64	0/4477
1	B	0.34	0/3316	0.71	3/4473 (0.1%)
1	C	0.30	0/3316	0.58	0/4473
1	D	0.30	0/3319	0.57	0/4477
1	E	0.29	0/3316	0.56	0/4473
1	F	0.31	0/3319	0.58	0/4477
All	All	0.32	0/19905	0.61	3/26850 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	SER	N-CA-C	-15.61	68.87	111.00
1	B	3	SER	CB-CA-C	11.18	131.33	110.10
1	B	4	LYS	N-CA-CB	-6.81	98.34	110.60

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	3256	0	3302	71	0
1	B	3253	0	3299	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3253	0	3299	126	0
1	D	3256	0	3302	118	0
1	E	3253	0	3299	113	0
1	F	3256	0	3302	101	0
2	A	10	0	4	1	0
2	B	10	0	4	3	0
2	C	10	0	4	1	0
2	D	10	0	4	3	0
2	E	10	0	4	1	0
2	F	10	0	4	2	0
3	A	392	0	0	13	0
3	B	328	0	0	10	0
3	C	167	0	0	9	0
3	D	151	0	0	4	0
3	E	130	0	0	1	0
3	F	205	0	0	8	0
All	All	20960	0	19827	581	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 15.

All (581) 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:D:117:ARG:H	1:D:370:GLN:HE22	1.00	0.98
1:A:7:VAL:HG21	1:A:38:VAL:HG13	1.46	0.96
1:D:79:PRO:HG3	1:D:93:TRP:HB2	1.51	0.92
1:C:117:ARG:HD2	1:C:370:GLN:HG2	1.51	0.92
1:F:206:LYS:HG3	1:F:244:LEU:HD23	1.52	0.90
1:C:360:ILE:HD12	1:C:409:ILE:HG12	1.54	0.90
1:D:7:VAL:HG21	1:D:38:VAL:HG22	1.54	0.90
1:B:161:ASP:OD1	1:B:163:THR:HG22	1.71	0.89
1:D:153:LEU:HD12	1:D:172:VAL:HB	1.56	0.88
1:C:213:THR:HG23	1:C:215:ASN:H	1.41	0.84
1:A:117:ARG:H	1:A:370:GLN:HE22	1.23	0.83
1:B:213:THR:HG23	1:B:215:ASN:H	1.42	0.83
1:C:80:ASP:OD1	1:C:83:ARG:HG2	1.80	0.82
1:D:117:ARG:N	1:D:370:GLN:HE22	1.79	0.79
1:B:7:VAL:HG21	1:B:38:VAL:HG12	1.63	0.79
1:B:2:PHE:C	1:B:3:SER:O	2.02	0.78
1:D:117:ARG:HB2	1:D:117:ARG:HH11	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:VAL:CG2	1:B:38:VAL:HG12	2.13	0.78
1:D:21:ARG:HH21	1:D:46:SER:HB3	1.48	0.78
1:B:137:GLY:N	3:B:2275:HOH:O	2.15	0.77
1:D:117:ARG:H	1:D:370:GLN:NE2	1.81	0.77
1:C:240:LYS:HE3	1:C:244:LEU:HD11	1.68	0.76
1:F:251:ARG:NH1	1:F:259:GLN:HE22	1.83	0.76
1:E:251:ARG:NH2	1:E:259:GLN:HE22	1.83	0.76
1:C:404:ARG:HA	1:C:407:LYS:HZ3	1.50	0.76
1:E:153:LEU:HD12	1:E:172:VAL:HB	1.68	0.76
1:B:213:THR:HG23	1:B:215:ASN:N	2.03	0.74
1:D:7:VAL:CG2	1:D:38:VAL:HG22	2.18	0.73
1:D:201:LEU:HD11	1:D:205:LYS:HD2	1.71	0.73
1:C:182:MET:HE1	1:D:218:LEU:HD13	1.70	0.72
1:D:356:LYS:HE2	1:D:412:ILE:HG12	1.70	0.72
1:B:393:THR:HG23	1:B:396:GLU:H	1.54	0.72
1:D:186:ASN:HD22	1:D:187:THR:H	1.35	0.72
1:E:387:GLU:HG2	1:E:390:ALA:HB2	1.72	0.72
1:B:117:ARG:H	1:B:370:GLN:HE22	1.37	0.72
1:E:7:VAL:HG21	1:E:38:VAL:HG12	1.72	0.71
1:A:48:GLU:HG2	1:C:29:LYS:HD3	1.72	0.70
1:F:388:ARG:HD3	1:F:388:ARG:O	1.91	0.70
1:C:136:HIS:CG	1:C:137:GLY:H	2.08	0.70
1:B:356:LYS:NZ	1:B:356:LYS:HB3	2.07	0.70
1:B:238:LYS:O	1:B:242:GLU:HG3	1.92	0.70
1:D:200:LYS:HE3	1:D:237:TYR:OH	1.91	0.70
1:A:7:VAL:CG2	1:A:38:VAL:HG13	2.22	0.69
1:C:343:LEU:O	1:C:347:GLU:HG3	1.93	0.69
1:D:388:ARG:HD3	1:D:388:ARG:O	1.92	0.69
1:E:369:VAL:HG13	1:E:375:MET:HB3	1.73	0.69
1:B:388:ARG:HD3	1:B:388:ARG:O	1.93	0.69
1:F:141:LYS:HA	1:F:141:LYS:HE2	1.74	0.69
1:F:360:ILE:HD12	1:F:361:LEU:N	2.08	0.69
1:B:393:THR:HG22	1:B:396:GLU:CG	2.24	0.68
1:E:117:ARG:H	1:E:370:GLN:HE22	1.39	0.68
1:C:213:THR:HG22	1:C:250:HIS:NE2	2.09	0.68
1:F:102:ASN:ND2	1:F:141:LYS:HD2	2.09	0.68
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.58	0.67
1:C:213:THR:HG23	1:C:215:ASN:N	2.09	0.67
1:E:145:THR:HA	1:F:220:LYS:HD2	1.77	0.66
1:E:101:ARG:HH22	2:E:2005:AKG:C1	2.08	0.66
1:F:19:MET:HG3	1:F:317:HIS:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:H	1:C:81:GLU:CD	1.98	0.66
1:E:262:LYS:HA	1:F:121:LEU:HD13	1.77	0.66
1:F:251:ARG:CZ	1:F:259:GLN:HE22	2.09	0.66
1:C:91:LYS:HG2	1:C:92:MET:N	2.11	0.65
1:C:123:PRO:HG2	1:D:123:PRO:HG2	1.79	0.65
1:D:371:GLN:NE2	1:D:404:ARG:HH22	1.95	0.64
1:A:319:ARG:NH1	1:A:323:LYS:HD2	2.12	0.64
1:B:406:GLN:O	1:B:409:ILE:HG22	1.96	0.64
1:F:127:LYS:HE2	1:F:266:GLY:HA3	1.80	0.64
1:C:220:LYS:HD2	1:D:144:ASP:O	1.97	0.64
1:C:405:LEU:O	1:C:409:ILE:HG13	1.97	0.64
1:C:117:ARG:CD	1:C:370:GLN:HG2	2.24	0.64
1:C:387:GLU:HG2	1:C:390:ALA:HB2	1.80	0.63
1:A:116:PRO:HB2	1:A:370:GLN:OE1	1.99	0.63
1:C:121:LEU:HD13	1:D:262:LYS:HA	1.80	0.63
1:E:301:ASP:OD1	1:E:303:LYS:HG2	1.97	0.63
1:E:395:GLU:CD	1:E:395:GLU:H	2.00	0.63
1:A:101:ARG:HH22	2:A:2001:AKG:C1	2.11	0.63
1:A:123:PRO:HG2	1:B:123:PRO:HG2	1.80	0.63
1:B:101:ARG:HH22	2:B:2002:AKG:C1	2.11	0.62
1:D:371:GLN:CD	1:D:404:ARG:HH22	2.03	0.62
1:B:31:LEU:C	1:B:32:ILE:HD12	2.20	0.62
1:F:297:LEU:HD23	1:F:298:VAL:N	2.14	0.62
1:C:101:ARG:HH22	2:C:2003:AKG:C1	2.12	0.62
1:C:136:HIS:CG	1:C:137:GLY:N	2.64	0.62
1:F:357:PHE:O	1:F:360:ILE:HG13	1.99	0.62
1:B:81:GLU:CD	1:B:81:GLU:H	2.03	0.62
1:D:356:LYS:O	1:D:360:ILE:HG23	1.99	0.61
1:B:388:ARG:HD3	1:B:388:ARG:C	2.21	0.61
1:E:14:LEU:CD2	1:E:61:ALA:HB1	2.31	0.61
1:E:7:VAL:CG2	1:E:38:VAL:HG12	2.30	0.61
1:D:153:LEU:HD12	1:D:172:VAL:CB	2.30	0.61
1:E:182:MET:HE1	1:F:218:LEU:HD13	1.81	0.61
1:D:387:GLU:OE2	1:D:389:SER:HB2	2.01	0.61
1:E:84:VAL:HG23	1:E:89:LEU:HB2	1.83	0.61
1:F:157:TYR:HB3	1:F:168:GLN:HB2	1.81	0.61
1:C:249:GLU:CD	1:C:251:ARG:HE	2.04	0.60
1:F:101:ARG:HH22	2:F:2006:AKG:C1	2.13	0.60
1:B:108:VAL:HG23	1:B:135:ALA:HB2	1.83	0.60
1:D:171:LYS:NZ	1:D:171:LYS:HB2	2.16	0.60
1:F:48:GLU:HG3	3:F:2015:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:TYR:O	1:B:322:GLN:HG2	2.02	0.60
1:C:252:LEU:HD11	1:C:254:ASP:OD2	2.01	0.60
1:C:201:LEU:HD12	1:C:268:ILE:CD1	2.32	0.60
1:E:388:ARG:HD3	1:E:388:ARG:O	2.01	0.60
1:F:201:LEU:HD13	1:F:205:LYS:HG3	1.84	0.60
1:D:21:ARG:NH2	1:D:46:SER:HB3	2.15	0.60
1:E:406:GLN:HA	1:E:409:ILE:HG22	1.84	0.60
1:E:108:VAL:HG23	1:E:135:ALA:HB2	1.83	0.59
1:E:397:PHE:O	1:E:401:VAL:HG23	2.00	0.59
1:B:1:ALA:O	1:B:3:SER:O	2.21	0.59
1:C:182:MET:CE	1:D:218:LEU:HD13	2.31	0.59
1:C:388:ARG:HD3	1:C:388:ARG:O	2.01	0.59
1:F:238:LYS:O	1:F:242:GLU:HG3	2.03	0.59
1:C:171:LYS:HD3	1:C:174:ASP:OD1	2.02	0.59
1:D:356:LYS:NZ	1:D:412:ILE:HA	2.17	0.59
1:F:131:ILE:HD12	1:F:280:SER:HA	1.84	0.59
1:A:121:LEU:HD13	1:B:262:LYS:HA	1.84	0.59
1:A:240:LYS:HG2	3:A:2342:HOH:O	2.03	0.58
1:B:136:HIS:CG	1:B:137:GLY:N	2.69	0.58
1:E:316:ARG:HA	1:E:319:ARG:HH12	1.68	0.58
1:E:201:LEU:HD12	1:E:268:ILE:HD13	1.85	0.58
1:A:32:ILE:N	1:A:32:ILE:HD12	2.18	0.58
1:D:201:LEU:CD1	1:D:205:LYS:HD2	2.33	0.58
1:D:19:MET:HG3	1:D:317:HIS:HB2	1.86	0.58
1:E:7:VAL:HG21	1:E:38:VAL:CG1	2.33	0.58
1:D:360:ILE:HD12	1:D:360:ILE:C	2.23	0.58
1:D:117:ARG:CB	1:D:117:ARG:HH11	2.14	0.58
2:D:2004:AKG:H31	3:D:2030:HOH:O	2.04	0.58
1:E:121:LEU:HD12	1:E:285:GLN:O	2.03	0.58
1:C:201:LEU:HD12	1:C:268:ILE:HD13	1.86	0.57
1:E:14:LEU:HD22	1:E:61:ALA:HB1	1.84	0.57
1:C:252:LEU:HD13	1:C:254:ASP:H	1.69	0.57
1:D:18:GLU:HB3	1:D:318:TYR:CG	2.39	0.57
1:D:30:LYS:HE2	1:D:30:LYS:HA	1.86	0.57
1:C:406:GLN:O	1:C:410:LYS:HG3	2.05	0.57
1:D:388:ARG:C	1:D:388:ARG:HD3	2.25	0.57
1:F:298:VAL:HG13	3:F:2160:HOH:O	2.05	0.57
1:D:117:ARG:HB2	1:D:117:ARG:NH1	2.18	0.57
1:C:66:LYS:HD2	3:C:2144:HOH:O	2.05	0.57
1:E:203:ILE:HD13	1:E:240:LYS:HG2	1.87	0.57
1:E:91:LYS:HG2	1:E:92:MET:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:PHE:CD2	1:F:251:ARG:HD2	2.39	0.57
1:B:3:SER:C	3:B:2175:HOH:O	2.43	0.56
1:C:404:ARG:HG2	1:C:404:ARG:HH11	1.71	0.56
1:D:124:ARG:O	1:D:126:GLU:HG3	2.04	0.56
1:D:90:HIS:O	1:D:91:LYS:HB2	2.05	0.56
1:C:209:LEU:HD12	1:C:248:TYR:CD1	2.41	0.56
1:E:116:PRO:HG2	1:E:370:GLN:OE1	2.05	0.56
1:B:36:LEU:HB3	1:B:38:VAL:HG13	1.88	0.56
1:B:403:LYS:O	1:B:407:LYS:HG2	2.05	0.56
1:D:187:THR:HG22	1:D:189:GLU:N	2.21	0.56
1:D:216:THR:HG23	1:D:252:LEU:HD21	1.87	0.56
1:F:211:LEU:HD12	1:F:250:HIS:HD2	1.70	0.56
1:C:251:ARG:HH12	1:C:259:GLN:CD	2.07	0.56
3:C:2110:HOH:O	1:D:187:THR:HG23	2.06	0.56
1:F:117:ARG:H	1:F:370:GLN:HE22	1.53	0.56
1:C:117:ARG:HD2	1:C:370:GLN:CG	2.30	0.56
1:D:230:GLN:O	1:D:234:GLU:HG3	2.05	0.56
1:E:409:ILE:HG23	1:E:410:LYS:HG3	1.87	0.56
1:F:18:GLU:HB3	1:F:318:TYR:CG	2.40	0.56
1:B:22:ILE:HD11	1:B:318:TYR:CE2	2.41	0.55
1:B:7:VAL:HG21	1:B:38:VAL:CG1	2.32	0.55
1:D:101:ARG:HH22	2:D:2004:AKG:C1	2.17	0.55
1:E:124:ARG:NH1	1:E:124:ARG:HB3	2.21	0.55
1:C:263:SER:HB2	3:C:2146:HOH:O	2.06	0.55
1:E:251:ARG:HH22	1:E:259:GLN:HE22	1.53	0.55
1:D:21:ARG:NH2	1:D:44:ASP:OD1	2.39	0.55
1:B:297:LEU:HD23	1:B:298:VAL:N	2.21	0.55
1:D:56:LYS:HE2	1:D:60:ASP:OD1	2.06	0.55
1:A:123:PRO:HG3	3:A:2253:HOH:O	2.07	0.55
1:B:319:ARG:HB2	1:B:319:ARG:HH11	1.72	0.55
1:B:393:THR:HG22	1:B:396:GLU:CD	2.27	0.55
1:F:111:GLU:HG3	3:F:2079:HOH:O	2.05	0.55
1:B:136:HIS:CG	1:B:137:GLY:H	2.23	0.55
1:D:108:VAL:HG23	1:D:135:ALA:HB2	1.89	0.55
1:B:213:THR:HG23	1:B:214:LYS:N	2.22	0.55
1:E:18:GLU:HB3	1:E:318:TYR:CG	2.41	0.55
1:F:7:VAL:HG21	1:F:38:VAL:HG22	1.89	0.55
1:D:301:ASP:OD1	1:D:303:LYS:HG2	2.07	0.55
1:B:24:TRP:CD2	1:B:74:CYS:HB2	2.42	0.54
1:F:108:VAL:HG23	1:F:135:ALA:HB2	1.88	0.54
1:F:395:GLU:N	1:F:395:GLU:OE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:HIS:C	3:B:2275:HOH:O	2.42	0.54
1:B:297:LEU:C	1:B:297:LEU:HD23	2.28	0.54
1:B:213:THR:HG21	1:B:215:ASN:HB3	1.88	0.54
1:A:139:GLN:HG3	1:A:184:MET:HE1	1.90	0.54
1:B:32:ILE:N	1:B:32:ILE:HD12	2.23	0.54
1:A:18:GLU:HB3	1:A:318:TYR:CG	2.43	0.54
1:D:87:PHE:HB2	1:D:89:LEU:HD11	1.88	0.54
1:F:200:LYS:HD2	3:F:2182:HOH:O	2.08	0.54
1:F:175:TYR:OH	1:F:181:ALA:HB2	2.08	0.53
1:F:388:ARG:HD3	1:F:388:ARG:C	2.29	0.53
1:E:124:ARG:HH11	1:E:124:ARG:CB	2.21	0.53
1:E:285:GLN:HG2	1:F:258:ALA:O	2.09	0.53
1:D:50:ARG:HD2	3:D:2035:HOH:O	2.08	0.53
1:A:153:LEU:HD21	1:B:155:LEU:HD22	1.89	0.53
1:C:224:ARG:HH11	1:C:224:ARG:HA	1.73	0.53
1:D:24:TRP:HH2	1:D:72:ILE:HG22	1.73	0.53
1:D:32:ILE:N	1:D:32:ILE:HD12	2.24	0.53
1:A:282:ILE:HD13	1:B:282:ILE:HD13	1.91	0.53
1:C:297:LEU:C	1:C:297:LEU:HD23	2.29	0.53
2:F:2006:AKG:H31	3:F:2085:HOH:O	2.09	0.53
1:B:316:ARG:HG3	1:B:317:HIS:N	2.23	0.53
1:C:262:LYS:HA	1:D:121:LEU:HD13	1.91	0.53
1:D:316:ARG:HG2	3:D:2139:HOH:O	2.08	0.53
1:E:117:ARG:HB2	1:E:370:GLN:NE2	2.24	0.52
1:F:27:ILE:HG22	1:F:32:ILE:HD13	1.91	0.52
1:B:326:GLU:CD	1:B:388:ARG:HH21	2.12	0.52
1:D:214:LYS:HG3	1:D:217:ILE:HD13	1.90	0.52
1:D:319:ARG:NH1	1:D:319:ARG:HB3	2.25	0.52
1:E:220:LYS:HD2	1:F:145:THR:HA	1.91	0.52
1:D:187:THR:HG22	1:D:189:GLU:H	1.75	0.52
1:D:31:LEU:C	1:D:32:ILE:HD12	2.30	0.52
1:B:22:ILE:HD11	1:B:318:TYR:HE2	1.75	0.52
1:C:220:LYS:HB3	1:D:146:LEU:HD12	1.92	0.52
1:A:377:LYS:O	1:A:381:LEU:HD13	2.10	0.52
1:C:260:MET:SD	1:C:269:MET:HE1	2.49	0.52
1:C:297:LEU:HD23	1:C:298:VAL:N	2.25	0.52
1:B:1:ALA:C	1:B:3:SER:O	2.47	0.52
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.75	0.52
1:F:83:ARG:NH1	1:F:83:ARG:HB2	2.24	0.51
1:A:206:LYS:HE2	3:A:2111:HOH:O	2.09	0.51
1:D:91:LYS:HG2	1:D:92:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:LYS:O	1:E:242:GLU:HG3	2.10	0.51
1:A:139:GLN:HG3	1:A:184:MET:CE	2.41	0.51
1:F:201:LEU:HD12	1:F:268:ILE:HD13	1.92	0.51
1:D:80:ASP:OD2	1:D:82:ALA:HB3	2.10	0.51
1:E:5:ILE:HB	1:E:36:LEU:HD23	1.93	0.51
1:F:188:ASP:O	1:F:192:GLU:HG3	2.10	0.51
1:F:314:VAL:HB	1:F:317:HIS:CD2	2.45	0.51
1:F:203:ILE:O	1:F:206:LYS:HD3	2.11	0.51
1:C:22:ILE:HD13	1:C:321:TYR:CD2	2.45	0.51
1:C:116:PRO:HG2	1:C:370:GLN:NE2	2.26	0.51
1:A:153:LEU:CD2	1:B:155:LEU:HD22	2.41	0.51
1:B:1:ALA:HB3	3:B:2175:HOH:O	2.10	0.51
1:C:175:TYR:OH	1:C:181:ALA:HB2	2.11	0.51
1:D:14:LEU:HD22	1:D:61:ALA:HB1	1.92	0.51
1:F:318:TYR:O	1:F:322:GLN:HG3	2.11	0.51
1:F:7:VAL:CG2	1:F:38:VAL:HG22	2.40	0.51
1:B:213:THR:HG22	1:B:250:HIS:NE2	2.25	0.51
1:D:395:GLU:CD	1:D:395:GLU:H	2.15	0.51
1:D:216:THR:OG1	1:D:217:ILE:HD12	2.10	0.50
1:A:117:ARG:HB3	1:A:370:GLN:HE22	1.77	0.50
1:A:254:ASP:HB3	1:B:281:ASP:OD1	2.10	0.50
1:E:138:ASP:HB3	1:E:139:GLN:OE1	2.11	0.50
1:F:85:LYS:NZ	1:F:85:LYS:HB2	2.26	0.50
1:C:153:LEU:HD12	1:C:172:VAL:HB	1.93	0.50
1:D:24:TRP:CH2	1:D:72:ILE:HG22	2.46	0.50
1:F:212:SER:OG	1:F:256:MET:HG2	2.12	0.50
1:E:121:LEU:HD13	1:F:262:LYS:HA	1.92	0.50
1:B:27:ILE:HG22	1:B:32:ILE:HD13	1.94	0.50
1:B:357:PHE:O	1:B:360:ILE:HG12	2.11	0.50
1:D:405:LEU:O	1:D:405:LEU:HD23	2.11	0.50
1:A:27:ILE:HG22	1:A:32:ILE:HD13	1.94	0.50
1:E:316:ARG:HG3	1:E:317:HIS:N	2.27	0.50
1:E:22:ILE:HD13	1:E:321:TYR:CE2	2.46	0.50
1:E:120:ARG:HD3	3:E:2111:HOH:O	2.12	0.49
1:E:251:ARG:CZ	1:E:259:GLN:HE22	2.25	0.49
1:E:314:VAL:HG12	1:E:316:ARG:HG2	1.94	0.49
1:A:298:VAL:HG13	3:A:2066:HOH:O	2.11	0.49
1:C:84:VAL:HG13	1:C:89:LEU:HB2	1.94	0.49
1:A:117:ARG:H	1:A:370:GLN:NE2	2.02	0.49
1:A:126:GLU:HG3	1:A:127:LYS:HG3	1.93	0.49
1:A:10:PRO:HG2	1:A:68:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLN:HG3	1:A:10:PRO:HD2	1.94	0.49
1:B:22:ILE:HD13	1:B:321:TYR:CD2	2.46	0.49
1:B:352:PRO:O	1:B:356:LYS:HG3	2.12	0.49
1:D:201:LEU:HD12	1:D:268:ILE:HD13	1.93	0.49
1:E:1:ALA:N	1:E:35:TYR:HB3	2.27	0.49
1:A:220:LYS:HD2	1:B:145:THR:HA	1.94	0.49
1:B:24:TRP:HH2	1:B:72:ILE:HG22	1.77	0.49
1:A:233:TYR:CE2	1:A:238:LYS:HD3	2.47	0.49
1:C:138:ASP:HB3	1:C:139:GLN:OE1	2.13	0.49
1:C:145:THR:HA	1:D:220:LYS:HD2	1.95	0.49
1:C:212:SER:OG	1:C:256:MET:HG2	2.13	0.49
1:D:19:MET:HG3	1:D:317:HIS:CB	2.43	0.49
1:E:220:LYS:CD	1:F:145:THR:HA	2.42	0.49
1:B:138:ASP:HB3	1:B:139:GLN:OE1	2.12	0.49
1:D:87:PHE:HB2	1:D:89:LEU:CD1	2.43	0.49
1:E:1:ALA:HB2	1:E:409:ILE:HD11	1.95	0.49
1:C:302:GLY:HA2	3:C:2023:HOH:O	2.13	0.49
1:F:201:LEU:HD12	1:F:268:ILE:CD1	2.43	0.49
1:C:153:LEU:HD21	1:D:155:LEU:CD1	2.43	0.48
1:C:284:ALA:HB3	1:C:290:LEU:HD23	1.95	0.48
1:D:262:LYS:HG2	1:D:262:LYS:O	2.13	0.48
1:F:31:LEU:C	1:F:32:ILE:HD12	2.33	0.48
1:A:387:GLU:HG3	3:A:2348:HOH:O	2.12	0.48
1:C:381:LEU:HA	1:C:385:ASN:O	2.13	0.48
1:E:1:ALA:HA	1:E:409:ILE:HG12	1.95	0.48
1:F:297:LEU:HD23	1:F:297:LEU:C	2.34	0.48
1:C:252:LEU:HD12	1:C:254:ASP:HB2	1.95	0.48
1:E:336:PHE:HA	1:E:339:SER:OG	2.13	0.48
1:C:14:LEU:HD22	1:C:61:ALA:HB1	1.94	0.48
1:C:340:ARG:NE	3:C:2143:HOH:O	2.47	0.48
1:C:24:TRP:CD2	1:C:74:CYS:HB2	2.48	0.48
1:C:153:LEU:HD21	1:D:155:LEU:HD11	1.95	0.48
1:C:117:ARG:HB3	1:C:117:ARG:NH1	2.29	0.48
1:D:147:ILE:HG13	1:D:175:TYR:CZ	2.49	0.48
1:D:187:THR:HG22	1:D:190:SER:H	1.78	0.48
1:E:32:ILE:N	1:E:32:ILE:HD12	2.29	0.48
1:F:251:ARG:NH1	1:F:259:GLN:NE2	2.59	0.48
1:A:121:LEU:HD12	1:A:285:GLN:HE21	1.79	0.48
1:B:393:THR:CG2	1:B:396:GLU:H	2.23	0.48
1:C:252:LEU:CD1	1:C:254:ASP:H	2.26	0.48
1:E:77:ILE:HG21	1:E:83:ARG:NE	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:HIS:HB3	3:A:2224:HOH:O	2.13	0.48
1:B:220:LYS:HD3	3:B:2035:HOH:O	2.13	0.48
1:D:406:GLN:O	1:D:409:ILE:HG22	2.14	0.48
1:F:210:PHE:HD2	1:F:251:ARG:HD2	1.76	0.48
1:E:381:LEU:HD23	1:E:386:ASN:HA	1.94	0.47
1:B:314:VAL:CG1	1:B:316:ARG:HG2	2.44	0.47
1:D:356:LYS:HZ3	1:D:412:ILE:HG23	1.79	0.47
1:E:319:ARG:NH1	1:E:319:ARG:HB3	2.29	0.47
1:F:301:ASP:CG	1:F:303:LYS:HG2	2.34	0.47
1:B:356:LYS:HZ2	1:B:356:LYS:HB3	1.76	0.47
1:C:117:ARG:HD2	1:C:370:GLN:HA	1.96	0.47
1:B:124:ARG:NH2	3:B:2055:HOH:O	2.47	0.47
1:C:213:THR:CG2	1:C:250:HIS:NE2	2.76	0.47
1:D:157:TYR:HB3	1:D:168:GLN:HB2	1.97	0.47
1:E:139:GLN:HA	1:E:142:ALA:HB2	1.95	0.47
1:F:240:LYS:O	1:F:244:LEU:HD13	2.15	0.47
1:B:319:ARG:HB2	1:B:319:ARG:NH1	2.29	0.47
1:C:117:ARG:NH1	1:C:383:CYS:SG	2.88	0.47
1:D:318:TYR:O	1:D:322:GLN:HG3	2.14	0.47
1:E:297:LEU:HD13	1:E:297:LEU:C	2.35	0.47
1:C:254:ASP:HB3	1:D:281:ASP:OD1	2.15	0.47
1:D:319:ARG:CZ	1:D:319:ARG:HB3	2.44	0.47
1:D:201:LEU:HD12	1:D:268:ILE:CD1	2.45	0.47
1:F:19:MET:HG3	1:F:317:HIS:CB	2.44	0.47
1:C:120:ARG:NH1	1:C:126:GLU:HA	2.30	0.47
1:C:393:THR:HG22	1:C:394:THR:N	2.29	0.47
1:D:171:LYS:HZ2	1:D:171:LYS:HB2	1.79	0.47
1:D:175:TYR:OH	1:D:181:ALA:HB2	2.15	0.47
1:E:32:ILE:HG23	1:E:36:LEU:HD12	1.97	0.47
1:F:196:HIS:O	1:F:200:LYS:HG3	2.15	0.47
1:F:295:SER:HB2	1:F:310:ALA:HB2	1.96	0.47
1:E:77:ILE:HG21	1:E:83:ARG:HE	1.80	0.47
1:F:150:PRO:HA	1:F:175:TYR:O	2.15	0.47
1:A:27:ILE:HG22	1:A:32:ILE:CD1	2.45	0.47
1:D:170:LEU:HD22	1:D:170:LEU:N	2.30	0.46
1:C:282:ILE:HD13	1:D:282:ILE:HD13	1.97	0.46
1:E:146:LEU:CD1	1:F:220:LYS:HB3	2.46	0.46
1:E:321:TYR:HD2	1:E:322:GLN:HE22	1.63	0.46
1:C:220:LYS:HD3	3:D:2097:HOH:O	2.15	0.46
1:D:89:LEU:N	1:D:89:LEU:HD12	2.31	0.46
1:F:201:LEU:CD1	1:F:205:LYS:HG3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:HG3	3:A:2074:HOH:O	2.14	0.46
1:C:153:LEU:HD11	1:D:155:LEU:HD21	1.97	0.46
1:A:402:GLU:O	1:A:406:GLN:HG3	2.15	0.46
1:C:18:GLU:HB3	1:C:318:TYR:CG	2.50	0.46
1:C:24:TRP:HH2	1:C:72:ILE:HG22	1.79	0.46
1:C:282:ILE:HG23	1:D:261:ILE:HG13	1.98	0.46
1:D:27:ILE:HG22	1:D:32:ILE:HD13	1.97	0.46
1:D:405:LEU:HD23	1:D:409:ILE:HB	1.97	0.46
1:E:124:ARG:HH11	1:E:124:ARG:HB3	1.80	0.46
1:E:131:ILE:HD13	1:E:269:MET:HB2	1.97	0.46
1:F:83:ARG:HB2	1:F:83:ARG:HH11	1.80	0.46
1:A:109:PHE:CE1	1:A:201:LEU:HD12	2.50	0.46
1:A:29:LYS:HE3	1:C:49:SER:HA	1.96	0.46
1:F:24:TRP:CD2	1:F:74:CYS:HB2	2.51	0.46
1:F:358:ALA:O	1:F:362:GLU:HG3	2.15	0.46
1:D:83:ARG:O	1:D:89:LEU:HD13	2.16	0.46
1:A:108:VAL:HG23	1:A:135:ALA:HB2	1.97	0.46
1:E:116:PRO:HG2	1:E:370:GLN:CD	2.37	0.46
1:A:203:ILE:HD11	1:A:241:PHE:CD1	2.51	0.46
1:A:224:ARG:CZ	1:A:228:ILE:HD11	2.46	0.46
1:B:147:ILE:HG13	1:B:175:TYR:CZ	2.51	0.46
1:B:393:THR:HG22	1:B:396:GLU:CB	2.46	0.46
1:D:16:GLY:N	1:D:74:CYS:HB3	2.31	0.46
1:A:360:ILE:CD1	1:A:409:ILE:HG13	2.45	0.45
1:C:116:PRO:CG	1:C:370:GLN:HE22	2.29	0.45
1:A:259:GLN:HG3	3:A:2248:HOH:O	2.15	0.45
1:E:153:LEU:HD12	1:E:172:VAL:CB	2.43	0.45
1:A:131:ILE:HD11	1:A:269:MET:HE3	1.96	0.45
1:C:203:ILE:HG23	1:C:244:LEU:HD11	1.97	0.45
1:F:214:LYS:HD3	1:F:252:LEU:HD11	1.96	0.45
1:E:212:SER:OG	1:E:256:MET:HG2	2.16	0.45
1:E:191:ILE:O	1:E:194:PHE:HB3	2.16	0.45
1:E:23:ILE:O	1:E:27:ILE:HG13	2.16	0.45
1:F:211:LEU:HD12	1:F:250:HIS:CD2	2.51	0.45
1:A:308:GLU:HG2	3:A:2134:HOH:O	2.17	0.45
1:E:212:SER:HA	1:E:251:ARG:O	2.17	0.45
1:F:115:ILE:HG12	1:F:366:LEU:HD22	1.99	0.45
1:F:134:HIS:HB2	1:F:194:PHE:CE1	2.52	0.45
1:E:182:MET:CE	1:F:218:LEU:HD13	2.44	0.45
1:C:161:ASP:O	1:C:163:THR:N	2.47	0.45
1:F:199:PHE:CZ	1:F:233:TYR:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASP:O	1:C:192:GLU:HG3	2.17	0.45
1:D:117:ARG:NH1	1:D:370:GLN:O	2.50	0.45
1:F:205:LYS:O	1:F:207:LEU:HG	2.17	0.45
1:F:32:ILE:N	1:F:32:ILE:HD12	2.32	0.45
1:E:117:ARG:N	1:E:370:GLN:HE22	2.08	0.44
1:B:213:THR:CG2	1:B:215:ASN:H	2.21	0.44
1:C:404:ARG:HA	1:C:407:LYS:NZ	2.26	0.44
1:F:301:ASP:OD1	1:F:303:LYS:HG2	2.17	0.44
1:D:356:LYS:HZ3	1:D:412:ILE:HA	1.81	0.44
1:E:196:HIS:O	1:E:200:LYS:HG3	2.17	0.44
1:A:24:TRP:CD2	1:A:74:CYS:HB2	2.52	0.44
1:A:14:LEU:HD22	1:A:61:ALA:HB1	1.98	0.44
1:C:116:PRO:HG2	1:C:370:GLN:HE22	1.82	0.44
1:D:118:ILE:HA	1:D:119:PRO:HD3	1.84	0.44
1:A:356:LYS:HE2	1:A:412:ILE:HD13	1.99	0.44
1:F:110:ARG:HD3	1:F:280:SER:OG	2.18	0.44
1:D:84:VAL:HA	1:D:89:LEU:HB2	2.00	0.44
1:E:5:ILE:HB	1:E:36:LEU:CD2	2.47	0.44
1:A:298:VAL:HG22	1:A:305:PHE:CD1	2.53	0.44
1:C:10:PRO:HB3	1:C:41:LYS:HE2	2.00	0.44
1:E:220:LYS:HB3	1:F:146:LEU:HD13	1.99	0.44
1:E:407:LYS:O	1:E:411:SER:HB3	2.18	0.44
1:F:295:SER:CB	1:F:310:ALA:HB2	2.47	0.44
1:F:50:ARG:HD2	3:F:2007:HOH:O	2.17	0.44
1:C:213:THR:HG23	1:C:214:LYS:N	2.32	0.44
1:E:81:GLU:O	1:E:84:VAL:HG12	2.17	0.44
1:F:230:GLN:HE21	1:F:234:GLU:HG3	1.83	0.44
1:A:224:ARG:O	1:A:228:ILE:HG12	2.18	0.44
1:C:393:THR:HG22	1:C:395:GLU:OE1	2.17	0.44
1:B:24:TRP:CH2	1:B:72:ILE:HG22	2.52	0.43
1:E:111:GLU:HB2	1:E:112:PRO:HD2	2.00	0.43
1:E:336:PHE:O	1:E:340:ARG:HG2	2.17	0.43
1:E:14:LEU:HD21	1:E:61:ALA:HB1	2.00	0.43
1:E:220:LYS:HD2	1:F:144:ASP:O	2.18	0.43
1:A:219:LYS:HE2	1:B:92:MET:CE	2.49	0.43
1:C:344:LYS:HE2	3:C:2149:HOH:O	2.18	0.43
1:E:202:ALA:HA	1:E:268:ILE:HD12	1.99	0.43
1:F:81:GLU:HA	1:F:81:GLU:OE1	2.19	0.43
1:A:224:ARG:NH2	1:A:228:ILE:HD11	2.33	0.43
1:C:212:SER:HA	1:C:251:ARG:O	2.18	0.43
1:C:91:LYS:HG2	1:C:92:MET:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.27	0.43
1:B:18:GLU:HB3	1:B:318:TYR:CG	2.54	0.43
1:B:14:LEU:HD22	1:B:61:ALA:HB1	2.01	0.43
1:C:36:LEU:HB3	1:C:38:VAL:HG22	1.99	0.43
1:B:81:GLU:HB2	3:B:2295:HOH:O	2.17	0.43
1:D:199:PHE:CZ	1:D:233:TYR:HB2	2.53	0.43
1:E:124:ARG:O	1:E:264:LYS:HA	2.18	0.43
1:E:316:ARG:HG3	1:E:317:HIS:HD2	1.84	0.43
1:F:24:TRP:CH2	1:F:72:ILE:HG22	2.54	0.43
1:A:120:ARG:NH1	3:A:2008:HOH:O	2.52	0.43
1:C:211:LEU:HD13	1:C:211:LEU:C	2.39	0.43
1:C:404:ARG:HG3	1:C:407:LYS:NZ	2.34	0.43
1:B:252:LEU:HD22	1:B:254:ASP:OD1	2.18	0.43
1:F:105:GLY:O	1:F:297:LEU:HD21	2.19	0.43
1:A:115:ILE:HG12	1:A:366:LEU:HD22	2.00	0.43
1:B:124:ARG:NH1	1:B:262:LYS:O	2.52	0.43
1:C:240:LYS:HE3	1:C:244:LEU:CD1	2.42	0.43
1:C:330:ASN:HB2	1:C:378:ASP:OD2	2.18	0.43
1:C:116:PRO:HD2	1:C:370:GLN:HE22	1.83	0.43
1:F:22:ILE:HD13	1:F:321:TYR:CD2	2.54	0.43
1:A:155:LEU:HD22	1:B:153:LEU:CD2	2.49	0.43
1:D:54:SER:HA	1:D:93:TRP:CH2	2.54	0.43
1:E:27:ILE:HG22	1:E:32:ILE:HD13	2.01	0.43
1:F:20:THR:OG1	1:F:313:THR:HB	2.18	0.43
1:A:183:ALA:HB2	1:B:155:LEU:HG	2.01	0.43
1:D:191:ILE:O	1:D:194:PHE:HB3	2.19	0.43
1:D:212:SER:HA	1:D:251:ARG:O	2.19	0.43
1:E:117:ARG:HB2	1:E:370:GLN:HE22	1.84	0.43
1:A:214:LYS:HD2	1:A:252:LEU:HD11	2.01	0.42
1:A:117:ARG:N	1:A:370:GLN:HE22	2.03	0.42
2:B:2002:AKG:H31	3:B:2312:HOH:O	2.18	0.42
1:C:131:ILE:HD13	1:C:269:MET:HB2	2.01	0.42
1:C:161:ASP:C	1:C:163:THR:H	2.21	0.42
1:C:213:THR:HG21	1:C:215:ASN:HB3	2.00	0.42
1:C:213:THR:OG1	1:C:222:ASP:HB3	2.18	0.42
1:E:377:LYS:HA	1:E:391:TYR:CD2	2.54	0.42
1:F:9:GLN:HG3	1:F:10:PRO:HD2	2.01	0.42
1:A:297:LEU:HB3	1:A:306:GLU:HB3	2.01	0.42
1:D:159:PRO:HD3	1:D:167:PRO:HA	2.01	0.42
1:F:262:LYS:HB3	1:F:262:LYS:NZ	2.33	0.42
1:B:125:TRP:CZ3	1:B:286:GLY:HA3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:O	1:C:194:PHE:HB3	2.19	0.42
1:D:314:VAL:HB	1:D:317:HIS:CD2	2.55	0.42
1:E:118:ILE:HA	1:E:119:PRO:HD3	1.84	0.42
1:E:81:GLU:C	1:E:84:VAL:HG12	2.40	0.42
1:F:53:THR:O	1:F:56:LYS:HB2	2.18	0.42
1:B:298:VAL:CG1	3:B:2277:HOH:O	2.66	0.42
1:B:393:THR:HG22	1:B:396:GLU:HB2	2.01	0.42
1:A:117:ARG:HB3	1:A:370:GLN:NE2	2.34	0.42
1:B:388:ARG:NH1	3:B:2159:HOH:O	2.53	0.42
1:E:111:GLU:HB3	1:E:130:ILE:HG12	2.02	0.42
1:A:31:LEU:C	1:A:32:ILE:HD12	2.39	0.42
1:B:211:LEU:HD13	1:B:250:HIS:HD2	1.83	0.42
1:C:274:TYR:HB3	3:C:2161:HOH:O	2.20	0.42
1:D:202:ALA:HA	1:D:268:ILE:HD12	2.01	0.42
1:E:155:LEU:CD2	1:F:153:LEU:HD21	2.50	0.42
1:F:360:ILE:C	1:F:360:ILE:HD12	2.40	0.42
1:A:360:ILE:HG13	1:A:361:LEU:N	2.33	0.42
1:B:393:THR:HG22	1:B:396:GLU:HG3	2.01	0.42
1:C:124:ARG:NH1	1:C:124:ARG:HB3	2.35	0.42
1:C:209:LEU:HD13	1:C:210:PHE:N	2.35	0.42
1:E:314:VAL:CG1	1:E:316:ARG:HG2	2.50	0.42
1:E:316:ARG:HG3	1:E:317:HIS:CD2	2.54	0.42
1:E:282:ILE:HD13	1:F:282:ILE:HD13	2.01	0.42
1:A:404:ARG:NH2	3:A:2170:HOH:O	2.52	0.42
1:B:314:VAL:HG12	1:B:316:ARG:HG2	2.02	0.42
1:C:136:HIS:O	1:C:273:ASN:ND2	2.53	0.42
1:C:77:ILE:HD13	1:C:83:ARG:CZ	2.50	0.42
1:E:253:ILE:O	1:E:257:VAL:HG22	2.19	0.42
1:B:110:ARG:NH1	2:B:2002:AKG:O2	2.53	0.41
1:C:158:LYS:HA	1:C:159:PRO:HD2	1.85	0.41
1:C:336:PHE:O	1:C:340:ARG:HG2	2.20	0.41
1:D:296:ILE:O	1:D:296:ILE:HG23	2.20	0.41
1:B:124:ARG:O	1:B:264:LYS:HA	2.20	0.41
1:B:117:ARG:N	1:B:370:GLN:HE22	2.11	0.41
1:C:124:ARG:NH1	1:C:262:LYS:O	2.52	0.41
1:E:274:TYR:HE1	1:F:214:LYS:HG3	1.86	0.41
1:A:120:ARG:HG3	3:A:2389:HOH:O	2.20	0.41
1:A:31:LEU:HB2	1:A:32:ILE:HD12	2.01	0.41
1:C:387:GLU:HG2	1:C:390:ALA:CB	2.49	0.41
1:C:50:ARG:HD2	3:C:2005:HOH:O	2.20	0.41
1:C:24:TRP:CH2	1:C:72:ILE:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:LYS:HE3	1:D:254:ASP:OD1	2.20	0.41
1:D:116:PRO:HB2	1:D:370:GLN:OE1	2.20	0.41
1:E:365:THR:HA	1:E:401:VAL:HG13	2.03	0.41
1:F:224:ARG:HD2	3:F:2035:HOH:O	2.20	0.41
1:F:32:ILE:HG23	1:F:36:LEU:HD12	2.02	0.41
1:A:147:ILE:HG13	1:A:175:TYR:CZ	2.55	0.41
1:C:121:LEU:HD12	1:C:285:GLN:HG3	2.03	0.41
1:C:377:LYS:HA	1:C:391:TYR:CD2	2.55	0.41
1:E:406:GLN:HA	1:E:409:ILE:CG2	2.50	0.41
1:B:121:LEU:HD12	1:B:285:GLN:O	2.20	0.41
1:C:260:MET:SD	1:C:269:MET:CE	3.09	0.41
1:E:155:LEU:CD1	1:F:153:LEU:HD21	2.50	0.41
1:F:319:ARG:HG3	1:F:319:ARG:HH11	1.85	0.41
1:C:159:PRO:C	1:C:161:ASP:H	2.24	0.41
1:C:166:GLN:HB3	1:C:167:PRO:HD2	2.03	0.41
1:C:387:GLU:CG	1:C:390:ALA:HB2	2.48	0.41
1:E:175:TYR:OH	1:E:181:ALA:HB2	2.19	0.41
1:F:298:VAL:HG22	1:F:305:PHE:CD1	2.56	0.41
1:B:356:LYS:HB3	1:B:356:LYS:HZ3	1.80	0.41
1:C:108:VAL:HG23	1:C:135:ALA:HB2	2.02	0.41
1:C:147:ILE:HG13	1:C:175:TYR:CZ	2.56	0.41
1:C:220:LYS:HB3	1:D:146:LEU:CD1	2.50	0.41
1:D:101:ARG:HH12	2:D:2004:AKG:C3	2.33	0.41
1:D:356:LYS:HZ1	1:D:412:ILE:HA	1.84	0.41
1:E:30:LYS:HB3	1:E:30:LYS:NZ	2.36	0.41
1:E:319:ARG:NH1	1:E:319:ARG:CB	2.82	0.41
1:F:118:ILE:HA	1:F:119:PRO:HD3	1.87	0.41
1:B:213:THR:CG2	1:B:250:HIS:NE2	2.84	0.41
1:B:338:TRP:O	1:B:342:LEU:HG	2.21	0.41
1:D:138:ASP:HB3	1:D:139:GLN:OE1	2.20	0.41
1:D:79:PRO:HG2	1:D:93:TRP:O	2.20	0.41
1:E:91:LYS:HG2	1:E:92:MET:H	1.84	0.41
1:F:117:ARG:H	1:F:370:GLN:NE2	2.18	0.41
1:C:124:ARG:O	1:C:264:LYS:HA	2.21	0.41
1:E:153:LEU:CD1	1:E:172:VAL:HB	2.44	0.41
1:E:28:LYS:HG2	1:E:33:LEU:HG	2.03	0.41
1:E:35:TYR:CD1	1:E:35:TYR:N	2.89	0.41
1:E:369:VAL:HG22	1:E:374:ILE:O	2.20	0.41
1:E:7:VAL:CB	1:E:38:VAL:HG12	2.51	0.41
1:C:159:PRO:C	1:C:161:ASP:N	2.74	0.41
1:C:388:ARG:HD3	1:C:388:ARG:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:NH1	1:D:319:ARG:CB	2.84	0.41
1:D:330:ASN:OD1	1:D:332:ILE:HG13	2.21	0.41
1:F:140:TYR:N	1:F:140:TYR:CD1	2.89	0.41
1:B:213:THR:CG2	1:B:215:ASN:HB3	2.48	0.41
1:D:319:ARG:HA	1:D:322:GLN:HE21	1.86	0.41
1:D:356:LYS:HD3	1:D:412:ILE:HG23	2.03	0.41
1:F:54:SER:HA	1:F:93:TRP:CH2	2.56	0.41
1:C:330:ASN:HD21	1:C:332:ILE:HB	1.85	0.40
1:D:212:SER:OG	1:D:256:MET:HG2	2.21	0.40
1:B:140:TYR:N	1:B:140:TYR:CD1	2.90	0.40
1:C:114:VAL:HG12	1:C:116:PRO:HD3	2.02	0.40
1:C:212:SER:HB3	1:C:253:ILE:HA	2.04	0.40
1:C:8:LYS:NZ	3:C:2135:HOH:O	2.53	0.40
1:D:32:ILE:N	1:D:32:ILE:CD1	2.85	0.40
1:D:33:LEU:HB2	1:D:34:PRO:HD3	2.03	0.40
1:E:316:ARG:HA	1:E:319:ARG:NH1	2.34	0.40
1:E:387:GLU:CG	1:E:390:ALA:HB2	2.48	0.40
1:A:260:MET:SD	1:A:269:MET:CE	3.09	0.40
1:B:20:THR:OG1	1:B:313:THR:HB	2.21	0.40
1:C:201:LEU:HD12	1:C:268:ILE:HD11	2.04	0.40
1:E:127:LYS:HA	1:E:128:PRO:HD3	1.95	0.40
1:F:124:ARG:HB2	3:F:2205:HOH:O	2.21	0.40
1:A:212:SER:HB3	1:A:253:ILE:HA	2.04	0.40
3:A:2122:HOH:O	1:B:92:MET:HE1	2.20	0.40
1:E:319:ARG:HH11	1:E:319:ARG:CB	2.34	0.40
1:E:335:ILE:CG2	1:E:361:LEU:HD22	2.52	0.40
1:E:4:LYS:HA	1:E:35:TYR:O	2.21	0.40
1:F:14:LEU:HD13	1:F:45:LEU:HD11	2.03	0.40
1:E:146:LEU:HD12	1:F:220:LYS:HB3	2.02	0.40
1:A:121:LEU:CD1	1:A:285:GLN:HE21	2.34	0.40
1:D:65:ILE:HD13	1:D:306:GLU:HG3	2.02	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	409/427 (96%)	395 (97%)	14 (3%)	0	100	100
1	B	409/427 (96%)	392 (96%)	15 (4%)	2 (0%)	29	26
1	C	409/427 (96%)	378 (92%)	25 (6%)	6 (2%)	10	5
1	D	409/427 (96%)	384 (94%)	23 (6%)	2 (0%)	29	26
1	E	409/427 (96%)	382 (93%)	23 (6%)	4 (1%)	15	11
1	F	409/427 (96%)	394 (96%)	13 (3%)	2 (0%)	29	26
All	All	2454/2562 (96%)	2325 (95%)	113 (5%)	16 (1%)	22	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	GLY
1	E	4	LYS
1	C	311	HIS
1	D	18	GLU
1	D	311	HIS
1	F	236	GLN
1	C	236	GLN
1	E	8	LYS
1	E	18	GLU
1	E	236	GLN
1	B	137	GLY
1	C	159	PRO
1	C	162	PRO
1	F	18	GLU
1	B	136	HIS
1	C	116	PRO

### 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	355/367 (97%)	341 (96%)	14 (4%)	32	33
1	B	354/367 (96%)	339 (96%)	15 (4%)	30	30
1	C	354/367 (96%)	343 (97%)	11 (3%)	40	43
1	D	355/367 (97%)	344 (97%)	11 (3%)	40	43
1	E	354/367 (96%)	344 (97%)	10 (3%)	43	47
1	F	355/367 (97%)	345 (97%)	10 (3%)	43	47
All	All	2127/2202 (97%)	2056 (97%)	71 (3%)	38	40

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	146	LEU
1	A	153	LEU
1	A	155	LEU
1	A	171	LYS
1	A	186	ASN
1	A	201	LEU
1	A	209	LEU
1	A	211	LEU
1	A	254	ASP
1	A	354	LEU
1	A	361	LEU
1	A	388	ARG
1	A	405	LEU
1	B	48	GLU
1	B	139	GLN
1	B	153	LEU
1	B	155	LEU
1	B	186	ASN
1	B	201	LEU
1	B	209	LEU
1	B	211	LEU
1	B	213	THR
1	B	252	LEU
1	B	254	ASP
1	B	354	LEU
1	B	361	LEU
1	B	388	ARG
1	B	405	LEU
1	C	9	GLN

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Mol	Chain	Res	Type
1	C	38	VAL
1	C	48	GLU
1	C	139	GLN
1	C	188	ASP
1	C	213	THR
1	C	224	ARG
1	C	247	HIS
1	C	343	LEU
1	C	354	LEU
1	C	361	LEU
1	D	6	LYS
1	D	117	ARG
1	D	171	LYS
1	D	186	ASN
1	D	209	LEU
1	D	211	LEU
1	D	254	ASP
1	D	303	LYS
1	D	354	LEU
1	D	361	LEU
1	D	388	ARG
1	E	81	GLU
1	E	139	GLN
1	E	206	LYS
1	E	209	LEU
1	E	211	LEU
1	E	252	LEU
1	E	293	MET
1	E	354	LEU
1	E	361	LEU
1	E	388	ARG
1	F	153	LEU
1	F	155	LEU
1	F	186	ASN
1	F	206	LYS
1	F	209	LEU
1	F	254	ASP
1	F	354	LEU
1	F	361	LEU
1	F	388	ARG
1	F	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	236	GLN
1	A	285	GLN
1	A	317	HIS
1	A	350	ASN
1	A	370	GLN
1	B	230	GLN
1	B	236	GLN
1	B	370	GLN
1	B	385	ASN
1	C	230	GLN
1	C	317	HIS
1	C	367	ASN
1	C	370	GLN
1	C	385	ASN
1	C	406	GLN
1	D	59	GLN
1	D	88	ASN
1	D	186	ASN
1	D	317	HIS
1	D	322	GLN
1	D	370	GLN
1	D	371	GLN
1	E	166	GLN
1	E	230	GLN
1	E	236	GLN
1	E	259	GLN
1	E	367	ASN
1	E	370	GLN
1	F	88	ASN
1	F	102	ASN
1	F	230	GLN
1	F	259	GLN
1	F	317	HIS
1	F	322	GLN
1	F	370	GLN
1	F	371	GLN
1	F	406	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 ⓘ

6 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	AKG	F	2006	-	3,9,9	1.03	0	4,11,11	0.86	0
2	AKG	B	2002	-	3,9,9	1.02	0	4,11,11	0.78	0
2	AKG	C	2003	-	3,9,9	1.06	0	4,11,11	0.67	0
2	AKG	D	2004	-	3,9,9	1.03	0	4,11,11	0.75	0
2	AKG	A	2001	-	3,9,9	1.07	0	4,11,11	0.77	0
2	AKG	E	2005	-	3,9,9	1.01	0	4,11,11	0.72	0

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	AKG	F	2006	-	-	2/3/9/9	-
2	AKG	B	2002	-	-	2/3/9/9	-
2	AKG	C	2003	-	-	2/3/9/9	-
2	AKG	D	2004	-	-	2/3/9/9	-
2	AKG	A	2001	-	-	2/3/9/9	-
2	AKG	E	2005	-	-	2/3/9/9	-

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2003	AKG	C1-C2-C3-C4
2	B	2002	AKG	C1-C2-C3-C4
2	B	2002	AKG	O5-C2-C3-C4
2	D	2004	AKG	C1-C2-C3-C4
2	A	2001	AKG	C1-C2-C3-C4
2	C	2003	AKG	O5-C2-C3-C4
2	E	2005	AKG	C1-C2-C3-C4
2	D	2004	AKG	O5-C2-C3-C4
2	A	2001	AKG	O5-C2-C3-C4
2	F	2006	AKG	C1-C2-C3-C4
2	E	2005	AKG	O5-C2-C3-C4
2	F	2006	AKG	O5-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2006	AKG	2	0
2	B	2002	AKG	3	0
2	C	2003	AKG	1	0
2	D	2004	AKG	3	0
2	A	2001	AKG	1	0
2	E	2005	AKG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	411/427 (96%)	0.21	8 (1%) 66 71	23, 34, 55, 89	0
1	B	411/427 (96%)	0.27	13 (3%) 47 54	21, 36, 65, 103	0
1	C	411/427 (96%)	0.63	37 (9%) 9 12	31, 48, 87, 103	0
1	D	411/427 (96%)	0.49	28 (6%) 17 21	34, 49, 89, 103	0
1	E	411/427 (96%)	0.73	49 (11%) 4 5	36, 53, 101, 128	0
1	F	411/427 (96%)	0.46	26 (6%) 20 24	31, 46, 73, 108	0
All	All	2466/2562 (96%)	0.46	161 (6%) 18 23	21, 45, 83, 128	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	19.1
1	E	2	PHE	10.1
1	C	2	PHE	9.9
1	A	2	PHE	8.0
1	F	412	ILE	7.9
1	E	3	SER	7.8
1	D	411	SER	7.5
1	B	411	SER	6.4
1	C	1	ALA	6.1
1	B	2	PHE	6.0
1	D	2	PHE	5.9
1	F	2	PHE	5.1
1	E	319	ARG	5.1
1	B	3	SER	5.1
1	C	162	PRO	5.0
1	D	410	LYS	4.9
1	E	386	ASN	4.9
1	C	291	GLY	4.8
1	E	390	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	4.6
1	F	247	HIS	4.3
1	E	381	LEU	4.3
1	D	412	ILE	4.3
1	A	412	ILE	4.2
1	E	387	GLU	4.2
1	C	313	THR	4.1
1	E	382	ALA	4.1
1	B	1	ALA	4.1
1	D	80	ASP	4.1
1	F	411	SER	4.1
1	C	385	ASN	4.0
1	E	410	LYS	3.9
1	D	387	GLU	3.9
1	D	85	LYS	3.9
1	C	386	ASN	3.8
1	C	390	ALA	3.8
1	C	381	LEU	3.8
1	E	409	ILE	3.7
1	D	323	LYS	3.7
1	E	384	GLY	3.7
1	E	411	SER	3.6
1	E	389	SER	3.6
1	B	319	ARG	3.6
1	C	319	ARG	3.6
1	F	246	ILE	3.5
1	D	87	PHE	3.5
1	C	384	GLY	3.5
1	C	388	ARG	3.5
1	C	166	GLN	3.4
1	E	323	LYS	3.4
1	F	3	SER	3.4
1	C	161	ASP	3.3
1	C	160	SER	3.3
1	E	391	TYR	3.3
1	E	369	VAL	3.3
1	D	406	GLN	3.2
1	C	391	TYR	3.2
1	E	320	LYS	3.2
1	D	319	ARG	3.2
1	D	386	ASN	3.2
1	B	410	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	156	VAL	3.1
1	E	388	ARG	3.1
1	C	3	SER	3.1
1	E	316	ARG	3.1
1	D	84	VAL	3.0
1	A	85	LYS	3.0
1	A	90	HIS	3.0
1	D	81	GLU	3.0
1	E	326	GLU	3.0
1	F	410	LYS	3.0
1	F	164	THR	2.9
1	E	84	VAL	2.9
1	E	311	HIS	2.9
1	C	240	LYS	2.9
1	F	278	VAL	2.8
1	A	319	ARG	2.8
1	C	86	GLU	2.8
1	F	242	GLU	2.8
1	E	385	ASN	2.8
1	C	242	GLU	2.8
1	D	3	SER	2.8
1	B	87	PHE	2.8
1	B	278	VAL	2.7
1	F	274	TYR	2.7
1	A	3	SER	2.7
1	A	278	VAL	2.7
1	D	390	ALA	2.7
1	C	85	LYS	2.7
1	E	237	TYR	2.6
1	C	314	VAL	2.6
1	D	317	HIS	2.6
1	D	409	ILE	2.6
1	E	399	ASP	2.6
1	B	274	TYR	2.6
1	E	278	VAL	2.6
1	C	164	THR	2.6
1	F	233	TYR	2.6
1	E	85	LYS	2.6
1	B	309	ALA	2.5
1	F	234	GLU	2.5
1	D	163	THR	2.5
1	F	238	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	165	ALA	2.5
1	E	317	HIS	2.5
1	B	312	GLY	2.5
1	F	165	ALA	2.5
1	E	325	GLU	2.5
1	C	310	ALA	2.5
1	F	244	LEU	2.4
1	E	274	TYR	2.4
1	F	82	ALA	2.4
1	E	403	LYS	2.4
1	D	316	ARG	2.4
1	C	238	LYS	2.4
1	C	244	LEU	2.4
1	C	410	LYS	2.4
1	A	274	TYR	2.4
1	F	271	LEU	2.3
1	D	90	HIS	2.3
1	C	246	ILE	2.3
1	F	409	ILE	2.3
1	F	309	ALA	2.3
1	E	360	ILE	2.3
1	B	140	TYR	2.3
1	C	165	ALA	2.3
1	F	235	ALA	2.3
1	C	118	ILE	2.3
1	C	241	PHE	2.3
1	C	411	SER	2.3
1	D	92	MET	2.2
1	D	243	GLN	2.2
1	D	314	VAL	2.2
1	E	314	VAL	2.2
1	B	407	LYS	2.2
1	E	406	GLN	2.1
1	E	165	ALA	2.1
1	E	242	GLU	2.1
1	C	290	LEU	2.1
1	E	4	LYS	2.1
1	E	378	ASP	2.1
1	C	278	VAL	2.1
1	C	383	CYS	2.1
1	E	407	LYS	2.1
1	C	382	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	310	ALA	2.1
1	F	311	HIS	2.1
1	E	6	LYS	2.1
1	E	246	ILE	2.1
1	D	407	LYS	2.1
1	E	376	THR	2.0
1	E	380	ALA	2.0
1	F	253	ILE	2.0
1	E	234	GLU	2.0
1	F	241	PHE	2.0
1	F	239	SER	2.0
1	F	243	GLN	2.0
1	E	253	ILE	2.0
1	E	366	LEU	2.0
1	E	405	LEU	2.0
1	D	278	VAL	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	AKG	E	2005	10/10	0.43	0.69	83,84,87,87	10
2	AKG	C	2003	10/10	0.58	0.74	75,77,80,80	10
2	AKG	F	2006	10/10	0.58	0.82	80,82,85,87	9
2	AKG	B	2002	10/10	0.60	0.68	76,77,80,80	10
2	AKG	D	2004	10/10	0.66	0.40	87,88,91,91	0
2	AKG	A	2001	10/10	0.72	0.37	72,74,76,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.