



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 AM GMT

PDB ID : 2QFY
Title : Crystal structure of *Saccharomyces cerevesiae* mitochondrial NADP(+)-dependent isocitrate dehydrogenase in complex with α -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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

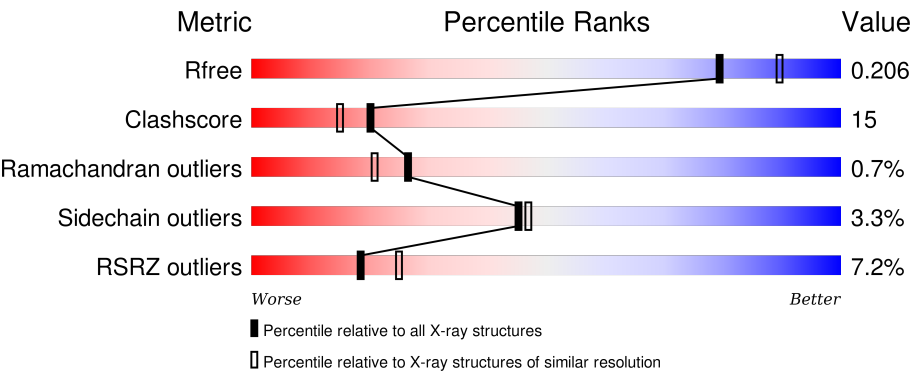
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 ≥ 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 $\leq 5\%$. 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>4%</div><div><div></div><div>75%</div><div>18%</div><div>• •</div></div></div>
1	C	427	<div><div>10%</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>13%</div><div><div></div><div>68%</div><div>26%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	427	

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	A	2001	-	-	-	X
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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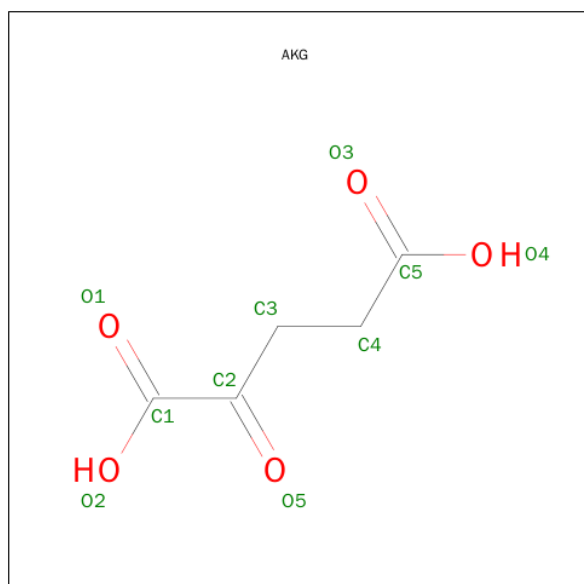
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP P21954
B	-9	HIS	-	EXPRESSION TAG	UNP P21954
B	-8	HIS	-	EXPRESSION TAG	UNP P21954
B	-7	HIS	-	EXPRESSION TAG	UNP P21954
B	-6	ALA	-	EXPRESSION TAG	UNP P21954
B	-5	MET	-	EXPRESSION TAG	UNP P21954
B	-4	GLY	-	EXPRESSION TAG	UNP 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: C₅H₆O₅).



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

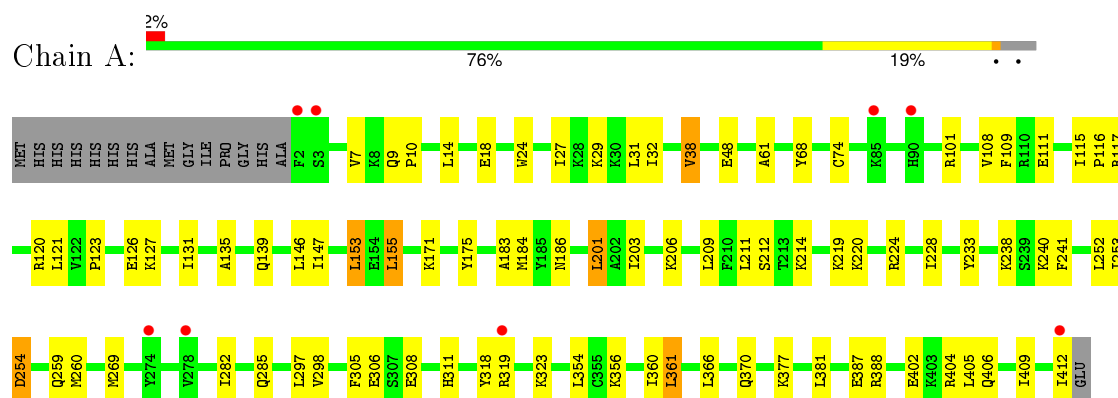
- Molecule 3 is water.

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

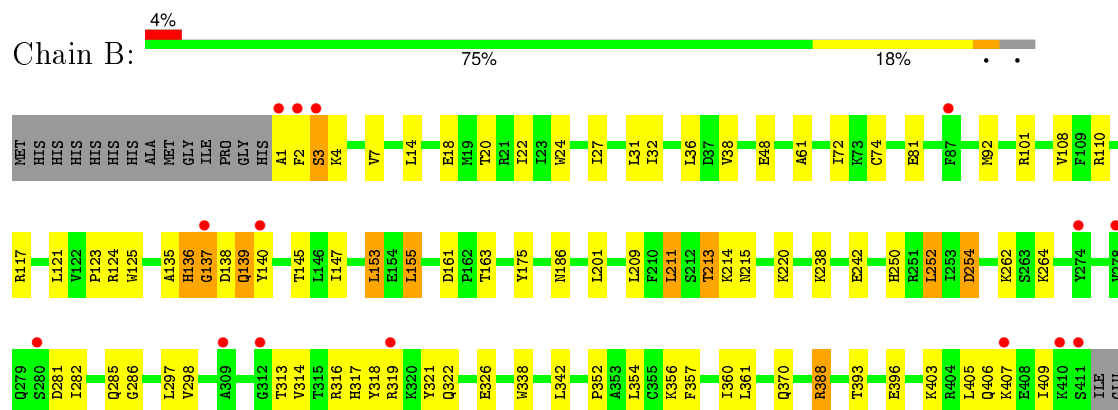
3 Residue-property plots

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.

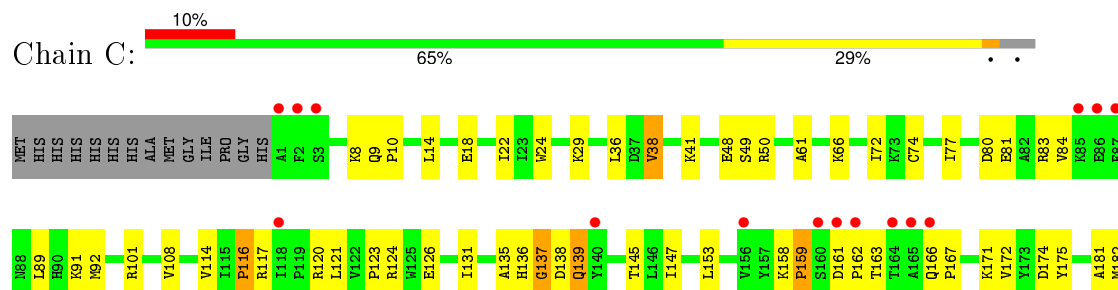
• Molecule 1: Isocitrate dehydrogenase [NADP]

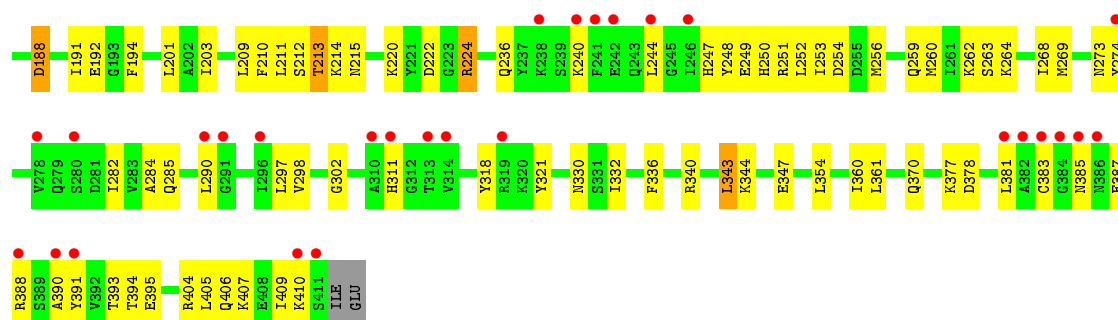


• Molecule 1: Isocitrate dehydrogenase [NADP]

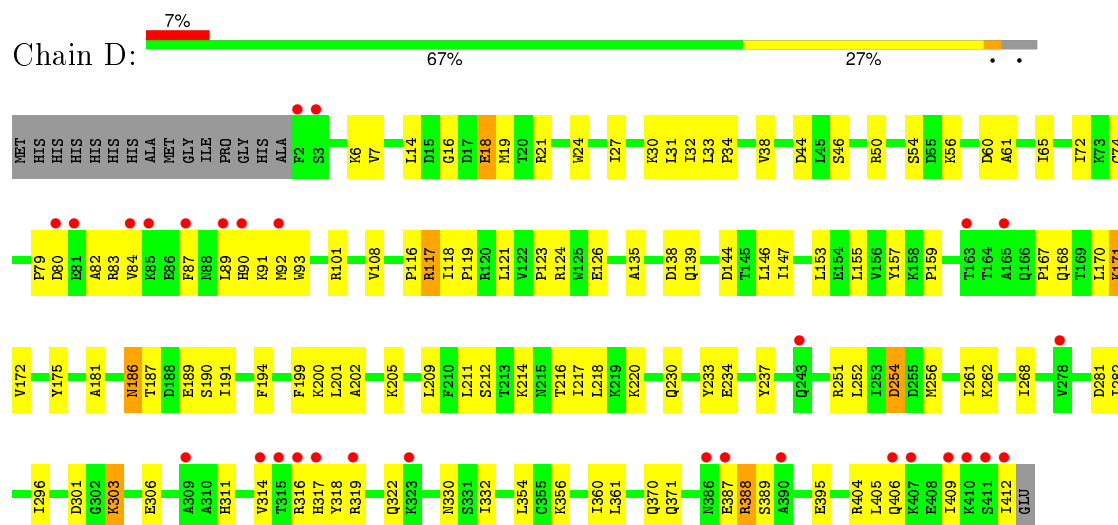


• Molecule 1: Isocitrate dehydrogenase [NADP]

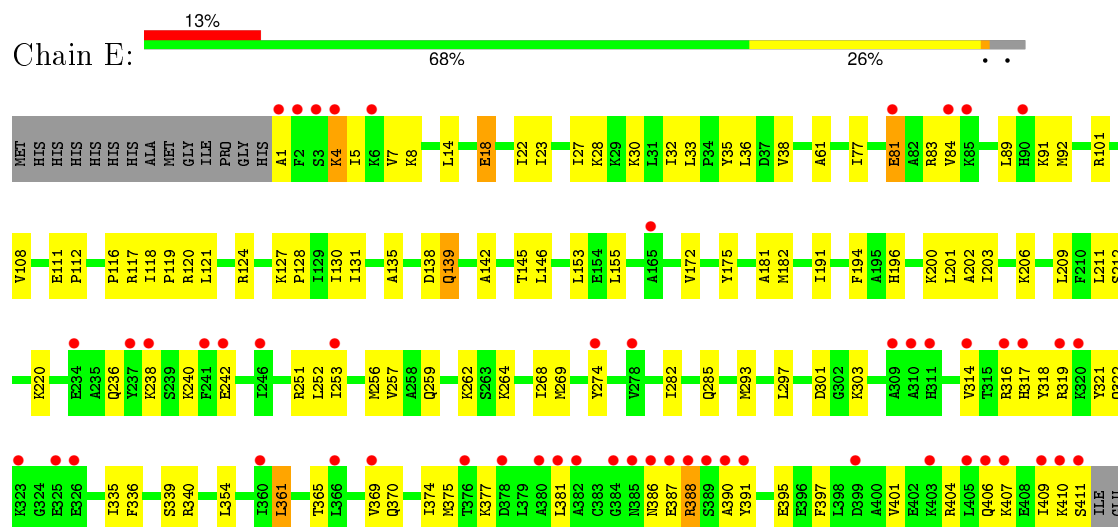




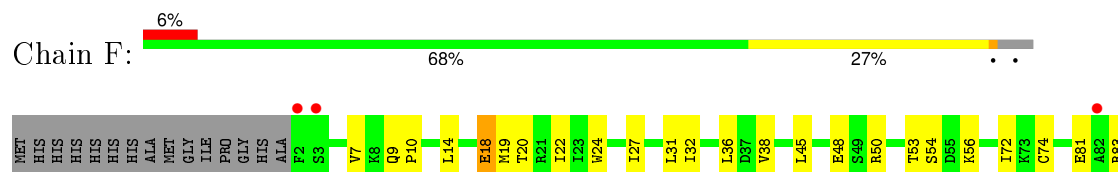
- Molecule 1: Isocitrate dehydrogenase [NADP]

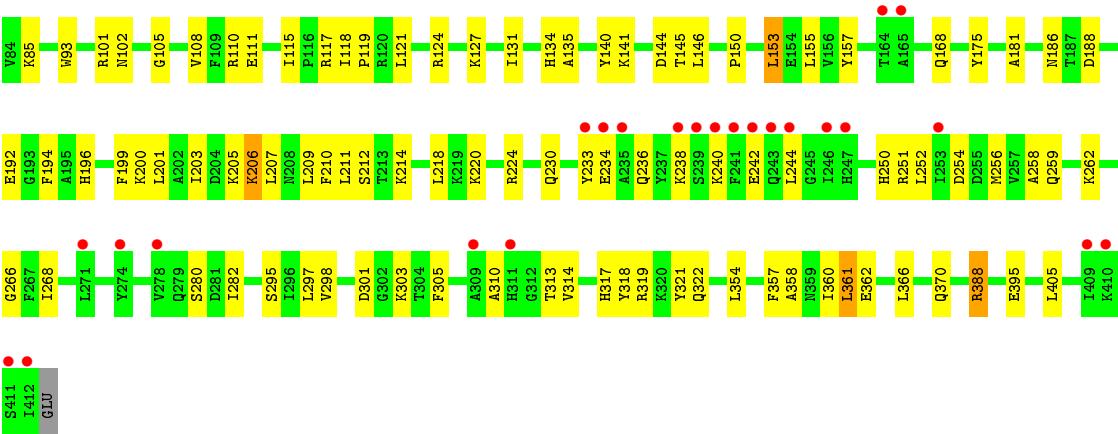


- Molecule 1: Isocitrate dehydrogenase [NADP]



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.08 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.247 0.208 , 0.206	Depositor DCC
R_{free} test set	7927 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.3	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 160557 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20960	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:D:117:ARG:HB2	1:D:117:ARG:HH11	1.46	0.78
1:B:2:PHE:C	1:B:3:SER:O	2.02	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:HB3	1:B:356:LYS:NZ	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:F:141:LYS:HA	1:F:141:LYS:HE2	1.74	0.69
1:B:388:ARG:HD3	1:B:388:ARG:O	1.93	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:C:213:THR:HG23	1:C:215:ASN:N	2.09	0.67
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.58	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:D:371:GLN:CD	1:D:404:ARG:HH22	2.03	0.62
1:B:101:ARG:HH22	2:B:2002:AKG:C1	2.11	0.62
1:F:297:LEU:HD23	1:F:298:VAL:N	2.14	0.62
1:B:31:LEU:C	1:B:32:ILE:HD12	2.20	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:C:101:ARG:HH22	2:C:2003:AKG:C1	2.12	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:E:7:VAL:CG2	1:E:38:VAL:HG12	2.30	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: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: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:D:387:GLU:OE2	1:D:389:SER:HB2	2.01	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:F:48:GLU:HG3	3:F:2015:HOH:O	2.02	0.60
1:D:171:LYS:NZ	1:D:171:LYS:HB2	2.16	0.60
1:B:108:VAL:HG23	1:B:135:ALA:HB2	1.83	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:F:201:LEU:HD13	1:F:205:LYS:HG3	1.84	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: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:F:238:LYS:O	1:F:242:GLU:HG3	2.03	0.59
1:C:388:ARG:HD3	1:C:388:ARG:O	2.01	0.59
1:D:356:LYS:NZ	1:D:412:ILE:HA	2.17	0.59
1:C:171:LYS:HD3	1:C:174:ASP:OD1	2.02	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:B:136:HIS:CG	1:B:137:GLY:N	2.69	0.58
1:A:240:LYS:HG2	3:A:2342:HOH:O	2.03	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:D:201:LEU:CD1	1:D:205:LYS:HD2	2.33	0.58
1:A:32:ILE:HD12	1:A:32:ILE:N	2.18	0.58
1:E:7:VAL:HG21	1:E:38:VAL:CG1	2.33	0.58
1:D:19:MET:HG3	1:D:317:HIS:HB2	1.86	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
1:E:121:LEU:HD12	1:E:285:GLN:O	2.03	0.58
2:D:2004:AKG:H31	3:D:2030:HOH:O	2.04	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:NH1	1:D:117:ARG:HB2	2.18	0.57
1:E:91:LYS:HG2	1:E:92:MET:N	2.20	0.57
1:E:203:ILE:HD13	1:E:240:LYS:HG2	1.87	0.57
1:C:66:LYS:HD2	3:C:2144:HOH:O	2.05	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:E:116:PRO:HG2	1:E:370:GLN:OE1	2.05	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:B:36:LEU:HB3	1:B:38:VAL:HG13	1.88	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:B:403:LYS:O	1:B:407:LYS:HG2	2.05	0.56
3:C:2110:HOH:O	1:D:187:THR:HG23	2.06	0.56
1:C:251:ARG:HH12	1:C:259:GLN:CD	2.07	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:E:409:ILE:HG23	1:E:410:LYS:HG3	1.87	0.56
1:D:230:GLN:O	1:D:234:GLU:HG3	2.05	0.56
1:F:18:GLU:HB3	1:F:318:TYR:CG	2.40	0.56
1:B:7:VAL:HG21	1:B:38:VAL:CG1	2.32	0.55
1:B:22:ILE:HD11	1:B:318:TYR:CE2	2.41	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:E:251:ARG:HH22	1:E:259:GLN:HE22	1.53	0.55
1:C:263:SER:HB2	3:C:2146:HOH:O	2.06	0.55
1:D:21:ARG:NH2	1:D:44:ASP:OD1	2.39	0.55
1:D:56:LYS:HE2	1:D:60:ASP:OD1	2.06	0.55
1:B:297:LEU:HD23	1:B:298:VAL:N	2.21	0.55
1:B:393:THR:HG22	1:B:396:GLU:CD	2.27	0.55
1:A:123:PRO:HG3	3:A:2253:HOH:O	2.07	0.55
1:F:111:GLU:HG3	3:F:2079:HOH:O	2.05	0.55
1:B:319:ARG:HB2	1:B:319:ARG:HH11	1.72	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:F:7:VAL:HG21	1:F:38:VAL:HG22	1.89	0.55
1:E:18:GLU:HB3	1:E:318:TYR:CG	2.41	0.55
1:D:301:ASP:OD1	1:D:303:LYS:HG2	2.07	0.55
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
1:B:24:TRP:CD2	1:B:74:CYS:HB2	2.42	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: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:A:18:GLU:HB3	1:A:318:TYR:CG	2.43	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:285:GLN:HG2	1:F:258:ALA:O	2.09	0.53
1:E:124:ARG:HH11	1:E:124:ARG:CB	2.21	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:HA	1:C:224:ARG:HH11	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
2:F:2006:AKG:H31	3:F:2085:HOH:O	2.09	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
1:B:316:ARG:HG3	1:B:317:HIS:N	2.23	0.53
1:D:316:ARG:HG2	3:D:2139:HOH:O	2.08	0.53
1:C:262:LYS:HA	1:D:121:LEU:HD13	1.91	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:319:ARG:NH1	1:D:319:ARG:HB3	2.25	0.52
1:D:214:LYS:HG3	1:D:217:ILE:HD13	1.90	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:C:220:LYS:HB3	1:D:146:LEU:HD12	1.92	0.52
1:B:22:ILE:HD11	1:B:318:TYR:HE2	1.75	0.52
1:C:297:LEU:HD23	1:C:298:VAL:N	2.25	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: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:D:91:LYS:HG2	1:D:92:MET:N	2.26	0.51
1:E:238:LYS:O	1:E:242:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HE2	3:A:2111:HOH:O	2.09	0.51
1:F:201:LEU:HD12	1:F:268:ILE:HD13	1.92	0.51
1:A:139:GLN:HG3	1:A:184:MET:CE	2.41	0.51
1:E:5:ILE:HB	1:E:36:LEU:HD23	1.93	0.51
1:D:80:ASP:OD2	1:D:82:ALA:HB3	2.10	0.51
1:F:314:VAL:HB	1:F:317:HIS:CD2	2.45	0.51
1:F:188:ASP:O	1:F:192:GLU:HG3	2.10	0.51
1:F:203:ILE:O	1:F:206:LYS:HD3	2.11	0.51
1:C:116:PRO:HG2	1:C:370:GLN:NE2	2.26	0.51
1:C:22:ILE:HD13	1:C:321:TYR:CD2	2.45	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: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: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: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:D:24:TRP:CH2	1:D:72:ILE:HG22	2.46	0.50
1:C:153:LEU:HD12	1:C:172:VAL:HB	1.93	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: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:E:120:ARG:HD3	3:E:2111:HOH:O	2.12	0.49
1:C:84:VAL:HG13	1:C:89:LEU:HB2	1.94	0.49
1:A:298:VAL:HG13	3:A:2066:HOH:O	2.11	0.49
1:A:117:ARG:H	1:A:370:GLN:NE2	2.02	0.49
1:D:201:LEU:HD12	1:D:268:ILE:HD13	1.93	0.49
1:B:352:PRO:O	1:B:356:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:HD13	1:B:321:TYR:CD2	2.46	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
1:A:9:GLN:HG3	1:A:10:PRO:HD2	1.94	0.49
1:E:1:ALA:N	1:E:35:TYR:HB3	2.27	0.49
1:B:24:TRP:HH2	1:B:72:ILE:HG22	1.77	0.49
1:A:220:LYS:HD2	1:B:145:THR:HA	1.94	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: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:A:233:TYR:CE2	1:A:238:LYS:HD3	2.47	0.49
1:E:1:ALA:HB2	1:E:409:ILE:HD11	1.95	0.49
1:D:87:PHE:HB2	1:D:89:LEU:CD1	2.43	0.49
1:B:138:ASP:HB3	1:B:139:GLN:OE1	2.12	0.49
1:F:201:LEU:HD12	1:F:268:ILE:CD1	2.43	0.49
1:C:302:GLY:HA2	3:C:2023:HOH:O	2.13	0.49
1:D:262:LYS:HG2	1:D:262:LYS:O	2.13	0.48
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:F:31:LEU:C	1:F:32:ILE:HD12	2.33	0.48
1:F:297:LEU:HD23	1:F:297:LEU:C	2.34	0.48
1:E:1:ALA:HA	1:E:409:ILE:HG12	1.95	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: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:340:ARG:NE	3:C:2143:HOH:O	2.47	0.48
1:C:14:LEU:HD22	1:C:61:ALA:HB1	1.94	0.48
1:C:153:LEU:HD21	1:D:155:LEU:HD11	1.95	0.48
1:C:24:TRP:CD2	1:C:74:CYS:HB2	2.48	0.48
1:C:117:ARG:NH1	1:C:117:ARG:HB3	2.29	0.48
1:F:251:ARG:NH1	1:F:259:GLN:NE2	2.59	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:D:147:ILE:HG13	1:D:175:TYR:CZ	2.49	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:A:121:LEU:HD12	1:A:285:GLN:HE21	1.79	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:F:210:PHE:HD2	1:F:251:ARG:HD2	1.76	0.48
1:D:406:GLN:O	1:D:409:ILE:HG22	2.14	0.48
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:E:381:LEU:HD23	1:E:386:ASN:HA	1.94	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:B:314:VAL:CG1	1:B:316:ARG:HG2	2.44	0.47
1:F:301:ASP:CG	1:F:303:LYS:HG2	2.34	0.47
1:C:117:ARG:HD2	1:C:370:GLN:HA	1.96	0.47
1:B:356:LYS:HB3	1:B:356:LYS:HZ2	1.76	0.47
1:F:240:LYS:O	1:F:244:LEU:HD13	2.15	0.47
1:C:213:THR:CG2	1:C:250:HIS:NE2	2.76	0.47
1:B:124:ARG:NH2	3:B:2055:HOH:O	2.47	0.47
1:E:139:GLN:HA	1:E:142:ALA:HB2	1.95	0.47
1:D:157:TYR:HB3	1:D:168:GLN:HB2	1.97	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:B:319:ARG:HB2	1:B:319:ARG:NH1	2.29	0.47
1:E:297:LEU:C	1:E:297:LEU:HD13	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:393:THR:HG22	1:C:394:THR:N	2.29	0.47
1:C:120:ARG:NH1	1:C:126:GLU:HA	2.30	0.47
1:D:171:LYS:HZ2	1:D:171:LYS:HB2	1.79	0.47
1:F:196:HIS:O	1:F:200:LYS:HG3	2.15	0.47
1:E:32:ILE:HG23	1:E:36:LEU:HD12	1.97	0.47
1:D:175:TYR:OH	1:D:181:ALA:HB2	2.15	0.47
1:F:295:SER:HB2	1:F:310:ALA:HB2	1.96	0.47
1:F:150:PRO:HA	1:F:175:TYR:O	2.15	0.47
1:E:77:ILE:HG21	1:E:83:ARG:HE	1.80	0.47
1:A:27:ILE:HG22	1:A:32:ILE:CD1	2.45	0.47
1:E:146:LEU:CD1	1:F:220:LYS:HB3	2.46	0.46
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: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:F:201:LEU:CD1	1:F:205:LYS:HG3	2.44	0.46
1:D:89:LEU:N	1:D:89:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:HD11	1:D:155:LEU:HD21	1.97	0.46
1:A:111:GLU:HG3	3:A:2074:HOH:O	2.14	0.46
1:E:124:ARG:HH11	1:E:124:ARG:HB3	1.80	0.46
1:D:27:ILE:HG22	1:D:32:ILE:HD13	1.97	0.46
1:F:83:ARG:HB2	1:F:83:ARG:HH11	1.80	0.46
1:D:405:LEU:HD23	1:D:409:ILE:HB	1.97	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:C:18:GLU:HB3	1:C:318:TYR:CG	2.50	0.46
1:E:131:ILE:HD13	1:E:269:MET:HB2	1.97	0.46
1:A:402:GLU:O	1:A:406:GLN:HG3	2.15	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:A:109:PHE:CE1	1:A:201:LEU:HD12	2.50	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:E:116:PRO:HG2	1:E:370:GLN:CD	2.37	0.46
1:A:108:VAL:HG23	1:A:135:ALA:HB2	1.97	0.46
1:B:393:THR:HG22	1:B:396:GLU:CB	2.46	0.46
1:B:147:ILE:HG13	1:B:175:TYR:CZ	2.51	0.46
1:D:16:GLY:N	1:D:74:CYS:HB3	2.31	0.46
1:A:224:ARG:CZ	1:A:228:ILE:HD11	2.46	0.46
1:A:203:ILE:HD11	1:A:241:PHE:CD1	2.51	0.46
1:C:116:PRO:CG	1:C:370:GLN:HE22	2.29	0.45
1:A:360:ILE:CD1	1:A:409:ILE:HG13	2.45	0.45
1:E:153:LEU:HD12	1:E:172:VAL:CB	2.43	0.45
1:A:259:GLN:HG3	3:A:2248:HOH:O	2.15	0.45
1:C:203:ILE:HG23	1:C:244:LEU:HD11	1.97	0.45
1:A:131:ILE:HD11	1:A:269:MET:HE3	1.96	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:F:211:LEU:HD12	1:F:250:HIS:CD2	2.51	0.45
1:E:23:ILE:O	1:E:27:ILE:HG13	2.16	0.45
1:E:191:ILE:O	1:E:194:PHE:HB3	2.16	0.45
1:E:212:SER:HA	1:E:251:ARG:O	2.17	0.45
1:E:182:MET:CE	1:F:218:LEU:HD13	2.44	0.45
1:A:308:GLU:HG2	3:A:2134:HOH:O	2.17	0.45
1:F:134:HIS:HB2	1:F:194:PHE:CE1	2.52	0.45
1:F:115:ILE:HG12	1:F:366:LEU:HD22	1.99	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: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:C:188:ASP:O	1:C:192:GLU:HG3	2.17	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: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: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:F:110:ARG:HD3	1:F:280:SER:OG	2.18	0.44
1:A:356:LYS:HE2	1:A:412:ILE:HD13	1.99	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:E:220:LYS:HB3	1:F:146:LEU:HD13	1.99	0.44
1:A:298:VAL:HG22	1:A:305:PHE:CD1	2.53	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:10:PRO:HB3	1:C:41:LYS:HE2	2.00	0.44
1:E:407:LYS:O	1:E:411:SER:HB3	2.18	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:C:393:THR:HG22	1:C:395:GLU:OE1	2.17	0.44
1:A:224:ARG:O	1:A:228:ILE:HG12	2.18	0.44
1:E:14:LEU:HD21	1:E:61:ALA:HB1	2.00	0.43
1:B:24:TRP:CH2	1:B:72:ILE:HG22	2.52	0.43
1:E:220:LYS:HD2	1:F:144:ASP:O	2.18	0.43
1:E:336:PHE:O	1:E:340:ARG:HG2	2.17	0.43
1:E:111:GLU:HB2	1:E:112:PRO:HD2	2.00	0.43
1:E:202:ALA:HA	1:E:268:ILE:HD12	1.99	0.43
1:C:344:LYS:HE2	3:C:2149:HOH:O	2.18	0.43
1:F:81:GLU:HA	1:F:81:GLU:OE1	2.19	0.43
1:A:219:LYS:HE2	1:B:92:MET:CE	2.49	0.43
1:C:91:LYS:HG2	1:C:92:MET:H	1.82	0.43
1:C:212:SER:HA	1:C:251:ARG:O	2.18	0.43
1:A:224:ARG:NH2	1:A:228:ILE:HD11	2.33	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:E:316:ARG:HG3	1:E:317:HIS:HD2	1.84	0.43
1:E:124:ARG:O	1:E:264:LYS:HA	2.18	0.43
1:F:24:TRP:CH2	1:F:72:ILE:HG22	2.54	0.43
1:D:199:PHE:CZ	1:D:233:TYR:HB2	2.53	0.43
1:C:404:ARG:HG3	1:C:407:LYS:NZ	2.34	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:F:105:GLY:O	1:F:297:LEU:HD21	2.19	0.43
1:B:252:LEU:HD22	1:B:254:ASP:OD1	2.18	0.43
1:C:116:PRO:HD2	1:C:370:GLN:HE22	1.83	0.43
1:C:240:LYS:HE3	1:C:244:LEU:CD1	2.42	0.43
1:B:124:ARG:NH1	1:B:262:LYS:O	2.52	0.43
1:C:330:ASN:HB2	1:C:378:ASP:OD2	2.18	0.43
1:A:115:ILE:HG12	1:A:366:LEU:HD22	2.00	0.43
1:F:22:ILE:HD13	1:F:321:TYR:CD2	2.54	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:A:155:LEU:HD22	1:B:153:LEU:CD2	2.49	0.43
1:F:20:THR:OG1	1:F:313:THR:HB	2.18	0.43
1:E:117:ARG:HB2	1:E:370:GLN:HE22	1.84	0.43
1:A:183:ALA:HB2	1:B:155:LEU:HG	2.01	0.43
1:D:212:SER:HA	1:D:251:ARG:O	2.19	0.43
1:D:191:ILE:O	1:D:194:PHE:HB3	2.19	0.43
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: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:A:214:LYS:HD2	1:A:252:LEU:HD11	2.01	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:F:262:LYS:HB3	1:F:262:LYS:NZ	2.33	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:E:81:GLU:C	1:E:84:VAL:HG12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:53:THR:O	1:F:56:LYS:HB2	2.18	0.42
1:B:125:TRP:CZ3	1:B:286:GLY:HA3	2.54	0.42
1:C:191:ILE:O	1:C:194:PHE:HB3	2.19	0.42
1:B:393:THR:HG22	1:B:396:GLU:HB2	2.01	0.42
1:B:298:VAL:CG1	3:B:2277:HOH:O	2.66	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:B:211:LEU:HD13	1:B:250:HIS:HD2	1.83	0.42
1:D:202:ALA:HA	1:D:268:ILE:HD12	2.01	0.42
1:F:360:ILE:C	1:F:360:ILE:HD12	2.40	0.42
1:A:31:LEU:C	1:A:32:ILE:HD12	2.39	0.42
1:C:274:TYR:HB3	3:C:2161:HOH:O	2.20	0.42
1:E:155:LEU:CD2	1:F:153:LEU:HD21	2.50	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:A:360:ILE:HG13	1:A:361:LEU:N	2.33	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:C:209:LEU:HD13	1:C:210:PHE:N	2.35	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:C:77:ILE:HD13	1:C:83:ARG:CZ	2.50	0.42
1:C:136:HIS:O	1:C:273:ASN:ND2	2.53	0.42
1:B:314:VAL:HG12	1:B:316:ARG:HG2	2.02	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:336:PHE:O	1:C:340:ARG:HG2	2.20	0.41
1:C:158:LYS:HA	1:C:159:PRO:HD2	1.85	0.41
1:D:296:ILE:O	1:D:296:ILE:HG23	2.20	0.41
1:B:117:ARG:N	1:B:370:GLN:HE22	2.11	0.41
1:B:124:ARG:O	1:B:264:LYS:HA	2.20	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:D:116:PRO:HB2	1:D:370:GLN:OE1	2.20	0.41
1:A:120:ARG:HG3	3:A:2389:HOH:O	2.20	0.41
1:C:387:GLU:HG2	1:C:390:ALA:CB	2.49	0.41
1:E:365:THR:HA	1:E:401:VAL:HG13	2.03	0.41
1:A:31:LEU:HB2	1:A:32:ILE:HD12	2.01	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:F:32:ILE:HG23	1:F:36:LEU:HD12	2.02	0.41
1:C:24:TRP:CH2	1:C:72:ILE:HG22	2.55	0.41
1:F:224:ARG:HD2	3:F:2035:HOH:O	2.20	0.41
1:C:50:ARG:HD2	3:C:2005:HOH:O	2.20	0.41
1:C:121:LEU:HD12	1:C:285:GLN:HG3	2.03	0.41
1:E:406:GLN:HA	1:E:409:ILE:CG2	2.50	0.41
1:C:377:LYS:HA	1:C:391:TYR:CD2	2.55	0.41
1:A:147:ILE:HG13	1:A:175:TYR:CZ	2.55	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:B:121:LEU:HD12	1:B:285:GLN:O	2.20	0.41
1:F:319:ARG:HH11	1:F:319:ARG:HG3	1.85	0.41
1:C:387:GLU:CG	1:C:390:ALA:HB2	2.48	0.41
1:F:298:VAL:HG22	1:F:305:PHE:CD1	2.56	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:E:175:TYR:OH	1:E:181:ALA:HB2	2.19	0.41
1:D:356:LYS:HZ1	1:D:412:ILE:HA	1.84	0.41
1:B:356:LYS:HB3	1:B:356:LYS:HZ3	1.80	0.41
1:C:220:LYS:HB3	1:D:146:LEU:CD1	2.50	0.41
1:E:319:ARG:NH1	1:E:319:ARG:CB	2.82	0.41
1:D:101:ARG:HH12	2:D:2004:AKG:C3	2.33	0.41
1:C:147:ILE:HG13	1:C:175:TYR:CZ	2.56	0.41
1:F:118:ILE:HA	1:F:119:PRO:HD3	1.87	0.41
1:E:30:LYS:HB3	1:E:30:LYS:NZ	2.36	0.41
1:C:108:VAL:HG23	1:C:135:ALA:HB2	2.02	0.41
1:D:79:PRO:HG2	1:D:93:TRP:O	2.20	0.41
1:B:213:THR:CG2	1:B:250:HIS:NE2	2.84	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: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:E:153:LEU:CD1	1:E:172:VAL:HB	2.44	0.41
1:E:7:VAL:CB	1:E:38:VAL:HG12	2.51	0.41
1:E:369:VAL:HG22	1:E:374:ILE:O	2.20	0.41
1:E:35:TYR:N	1:E:35:TYR:CD1	2.89	0.41
1:C:388:ARG:HD3	1:C:388:ARG:C	2.41	0.41
1:D:319:ARG:NH1	1:D:319:ARG:CB	2.84	0.41
1:C:124:ARG:O	1:C:264:LYS:HA	2.21	0.41
1:C:159:PRO:C	1:C:161:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LYS:HG2	1:E:33:LEU:HG	2.03	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:356:LYS:HD3	1:D:412:ILE:HG23	2.03	0.41
1:D:319:ARG:HA	1:D:322:GLN:HE21	1.86	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:C:114:VAL:HG12	1:C:116:PRO:HD3	2.02	0.40
1:E:387:GLU:CG	1:E:390:ALA:HB2	2.48	0.40
1:C:212:SER:HB3	1:C:253:ILE:HA	2.04	0.40
1:E:316:ARG:HA	1:E:319:ARG:NH1	2.34	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:B:140:TYR:N	1:B:140:TYR:CD1	2.90	0.40
1:C:8:LYS:NZ	3:C:2135:HOH:O	2.53	0.40
1:C:201:LEU:HD12	1:C:268:ILE:HD11	2.04	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: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:E:146:LEU:HD12	1:F:220:LYS:HB3	2.02	0.40
1:E:4:LYS:HA	1:E:35:TYR:O	2.21	0.40
1:E:319:ARG:HH11	1:E:319:ARG:CB	2.34	0.40
3:A:2122:HOH:O	1:B:92:MET:HE1	2.20	0.40
1:A:212:SER:HB3	1:A:253:ILE:HA	2.04	0.40
1:F:14:LEU:HD13	1:F:45:LEU:HD11	2.03	0.40
1:E:335:ILE:CG2	1:E:361:LEU:HD22	2.52	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 ⓘ

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	409/427 (96%)	395 (97%)	14 (3%)	0	100	100
1	B	409/427 (96%)	392 (96%)	15 (4%)	2 (0%)	34	30
1	C	409/427 (96%)	378 (92%)	25 (6%)	6 (2%)	13	7
1	D	409/427 (96%)	384 (94%)	23 (6%)	2 (0%)	34	30
1	E	409/427 (96%)	382 (93%)	23 (6%)	4 (1%)	19	13
1	F	409/427 (96%)	394 (96%)	13 (3%)	2 (0%)	34	30
All	All	2454/2562 (96%)	2325 (95%)	113 (5%)	16 (1%)	26	21

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%)	39	39
1	B	354/367 (96%)	339 (96%)	15 (4%)	36	35
1	C	354/367 (96%)	343 (97%)	11 (3%)	47	50
1	D	355/367 (97%)	344 (97%)	11 (3%)	47	50
1	E	354/367 (96%)	344 (97%)	10 (3%)	51	55
1	F	355/367 (97%)	345 (97%)	10 (3%)	51	55
All	All	2127/2202 (97%)	2056 (97%)	71 (3%)	45	47

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	A	2001	-	3,9,9	1.01	0	4,11,11	0.72	0
2	AKG	B	2002	-	3,9,9	0.96	0	4,11,11	0.72	0
2	AKG	C	2003	-	3,9,9	0.99	0	4,11,11	0.63	0
2	AKG	D	2004	-	3,9,9	0.97	0	4,11,11	0.70	0
2	AKG	E	2005	-	3,9,9	0.95	0	4,11,11	0.66	0
2	AKG	F	2006	-	3,9,9	0.96	0	4,11,11	0.81	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	A	2001	-	-	0/3/9/9	0/0/0/0
2	AKG	B	2002	-	-	0/3/9/9	0/0/0/0
2	AKG	C	2003	-	-	0/3/9/9	0/0/0/0
2	AKG	D	2004	-	-	0/3/9/9	0/0/0/0
2	AKG	E	2005	-	-	0/3/9/9	0/0/0/0
2	AKG	F	2006	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	AKG	1	0
2	B	2002	AKG	3	0
2	C	2003	AKG	1	0
2	D	2004	AKG	3	0
2	E	2005	AKG	1	0
2	F	2006	AKG	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/427 (96%)	0.27	8 (1%) 70 75	23, 34, 55, 89	0
1	B	411/427 (96%)	0.34	15 (3%) 46 55	21, 36, 65, 103	0
1	C	411/427 (96%)	0.70	43 (10%) 8 11	31, 48, 87, 103	0
1	D	411/427 (96%)	0.56	30 (7%) 18 24	34, 49, 89, 103	0
1	E	411/427 (96%)	0.81	54 (13%) 5 6	36, 53, 101, 128	0
1	F	411/427 (96%)	0.53	27 (6%) 22 29	31, 46, 73, 108	0
All	All	2466/2562 (96%)	0.53	177 (7%) 18 25	21, 45, 83, 128	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	20.0
1	E	2	PHE	10.5
1	C	2	PHE	10.4
1	F	412	ILE	8.4
1	A	2	PHE	8.4
1	E	3	SER	8.1
1	D	411	SER	7.7
1	B	411	SER	6.6
1	C	1	ALA	6.5
1	B	2	PHE	6.4
1	D	2	PHE	6.2
1	F	2	PHE	5.4
1	E	319	ARG	5.3
1	B	3	SER	5.3
1	C	162	PRO	5.2
1	D	410	LYS	5.1
1	E	390	ALA	5.0
1	C	291	GLY	5.0
1	E	386	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	4.8
1	D	412	ILE	4.6
1	E	381	LEU	4.5
1	A	412	ILE	4.5
1	F	247	HIS	4.4
1	E	382	ALA	4.4
1	B	1	ALA	4.3
1	C	313	THR	4.3
1	E	387	GLU	4.3
1	D	80	ASP	4.3
1	F	411	SER	4.3
1	C	385	ASN	4.2
1	C	390	ALA	4.1
1	C	381	LEU	4.0
1	E	410	LYS	4.0
1	E	409	ILE	4.0
1	D	85	LYS	4.0
1	D	387	GLU	4.0
1	C	386	ASN	4.0
1	E	384	GLY	3.9
1	D	323	LYS	3.8
1	E	411	SER	3.8
1	F	246	ILE	3.8
1	E	389	SER	3.7
1	D	87	PHE	3.7
1	C	319	ARG	3.7
1	B	319	ARG	3.7
1	C	384	GLY	3.6
1	E	323	LYS	3.6
1	F	3	SER	3.6
1	C	388	ARG	3.6
1	C	166	GLN	3.6
1	E	369	VAL	3.5
1	C	161	ASP	3.5
1	C	160	SER	3.4
1	E	391	TYR	3.4
1	C	156	VAL	3.4
1	D	406	GLN	3.4
1	C	391	TYR	3.4
1	E	320	LYS	3.3
1	D	319	ARG	3.3
1	D	386	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	410	LYS	3.3
1	D	84	VAL	3.3
1	C	3	SER	3.3
1	E	388	ARG	3.2
1	E	316	ARG	3.2
1	E	84	VAL	3.1
1	A	85	LYS	3.1
1	F	164	THR	3.1
1	A	90	HIS	3.1
1	D	81	GLU	3.1
1	E	326	GLU	3.1
1	F	278	VAL	3.1
1	F	410	LYS	3.1
1	E	311	HIS	3.0
1	A	319	ARG	3.0
1	B	278	VAL	3.0
1	C	240	LYS	3.0
1	B	87	PHE	2.9
1	C	86	GLU	2.9
1	F	242	GLU	2.9
1	A	278	VAL	2.9
1	E	385	ASN	2.9
1	D	3	SER	2.9
1	C	242	GLU	2.9
1	C	314	VAL	2.9
1	D	390	ALA	2.9
1	F	274	TYR	2.9
1	A	3	SER	2.8
1	D	409	ILE	2.8
1	E	278	VAL	2.8
1	E	399	ASP	2.8
1	E	237	TYR	2.8
1	D	317	HIS	2.8
1	C	85	LYS	2.8
1	C	164	THR	2.8
1	B	274	TYR	2.7
1	B	309	ALA	2.7
1	D	165	ALA	2.7
1	F	233	TYR	2.7
1	D	163	THR	2.7
1	E	85	LYS	2.7
1	F	165	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	234	GLU	2.6
1	C	310	ALA	2.6
1	B	312	GLY	2.6
1	F	244	LEU	2.6
1	F	238	LYS	2.6
1	F	82	ALA	2.6
1	E	317	HIS	2.6
1	E	325	GLU	2.5
1	E	274	TYR	2.5
1	C	244	LEU	2.5
1	E	403	LYS	2.5
1	F	271	LEU	2.5
1	C	246	ILE	2.5
1	D	316	ARG	2.5
1	F	409	ILE	2.5
1	C	238	LYS	2.5
1	E	360	ILE	2.5
1	F	309	ALA	2.5
1	A	274	TYR	2.5
1	C	118	ILE	2.5
1	C	410	LYS	2.5
1	C	165	ALA	2.4
1	F	235	ALA	2.4
1	D	90	HIS	2.4
1	C	241	PHE	2.4
1	B	140	TYR	2.4
1	C	411	SER	2.4
1	D	314	VAL	2.4
1	E	314	VAL	2.4
1	D	92	MET	2.3
1	E	165	ALA	2.3
1	D	243	GLN	2.3
1	C	278	VAL	2.3
1	C	290	LEU	2.3
1	B	407	LYS	2.3
1	C	382	ALA	2.3
1	E	406	GLN	2.2
1	E	246	ILE	2.2
1	E	310	ALA	2.2
1	E	378	ASP	2.2
1	C	383	CYS	2.2
1	E	242	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	4	LYS	2.2
1	F	253	ILE	2.2
1	E	380	ALA	2.2
1	D	278	VAL	2.2
1	E	253	ILE	2.2
1	E	407	LYS	2.2
1	E	376	THR	2.2
1	F	311	HIS	2.2
1	F	241	PHE	2.2
1	E	6	LYS	2.2
1	E	366	LEU	2.1
1	E	405	LEU	2.1
1	D	407	LYS	2.1
1	F	239	SER	2.1
1	B	280	SER	2.1
1	C	296	ILE	2.1
1	D	315	THR	2.1
1	E	234	GLU	2.1
1	F	243	GLN	2.1
1	D	309	ALA	2.1
1	C	87	PHE	2.1
1	E	241	PHE	2.1
1	C	140	TYR	2.1
1	E	309	ALA	2.0
1	E	81	GLU	2.0
1	C	274	TYR	2.0
1	E	238	LYS	2.0
1	F	240	LYS	2.0
1	C	311	HIS	2.0
1	B	137	GLY	2.0
1	C	280	SER	2.0
1	E	90	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	AKG	B	2002	10/10	0.60	0.68	15.15	76,77,80,80	10
2	AKG	E	2005	10/10	0.43	0.69	14.19	83,84,87,87	10
2	AKG	C	2003	10/10	0.58	0.74	13.90	75,77,80,80	10
2	AKG	F	2006	10/10	0.58	0.82	13.84	80,82,85,87	9
2	AKG	D	2004	10/10	0.66	0.40	7.88	87,88,91,91	0
2	AKG	A	2001	10/10	0.72	0.37	6.62	72,74,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.