



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 2QFY / pdb_00002qfy
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

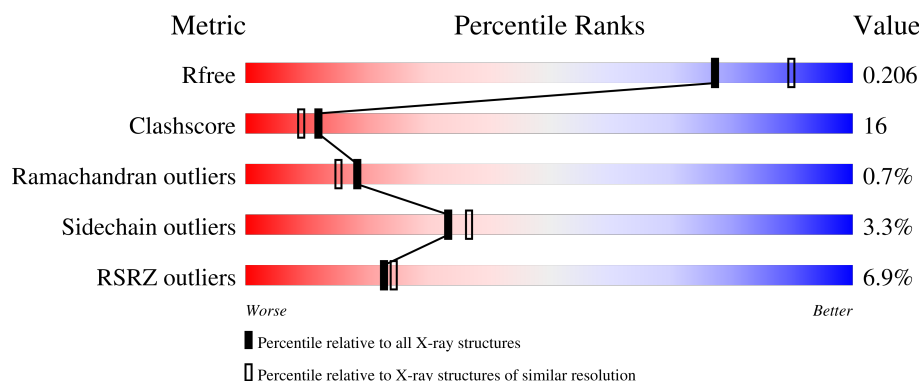
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 72% 22% • •
1	B	427	4% 72% 22% • •
1	C	427	10% 64% 30% • •
1	D	427	9% 65% 29% • •
1	E	427	9% 67% 28% • •

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Mol	Chain	Length	Quality of chain
1	F	427	6% 65% 29%

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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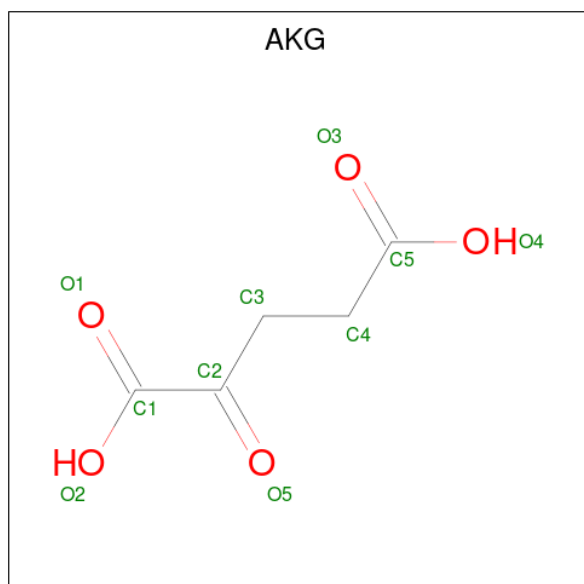
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP P21954
B	-9	HIS	-	expression tag	UNP P21954
B	-8	HIS	-	expression tag	UNP P21954
B	-7	HIS	-	expression tag	UNP P21954
B	-6	ALA	-	expression tag	UNP P21954
B	-5	MET	-	expression tag	UNP P21954
B	-4	GLY	-	expression tag	UNP 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 (CCD ID: AKG) (formula: C₅H₆O₅).



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

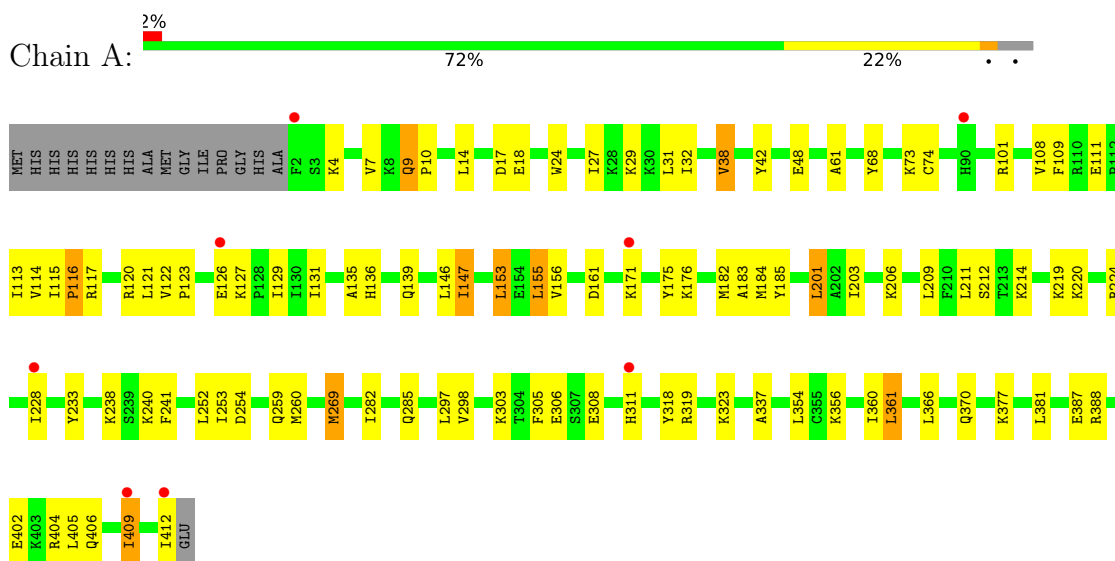
- Molecule 3 is water.

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

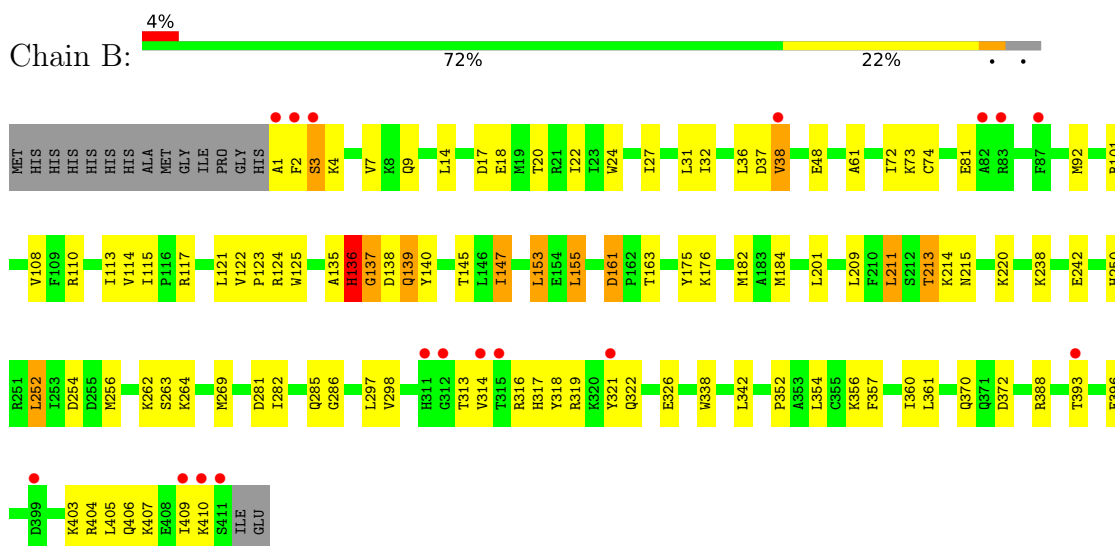
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Isocitrate dehydrogenase [NADP]

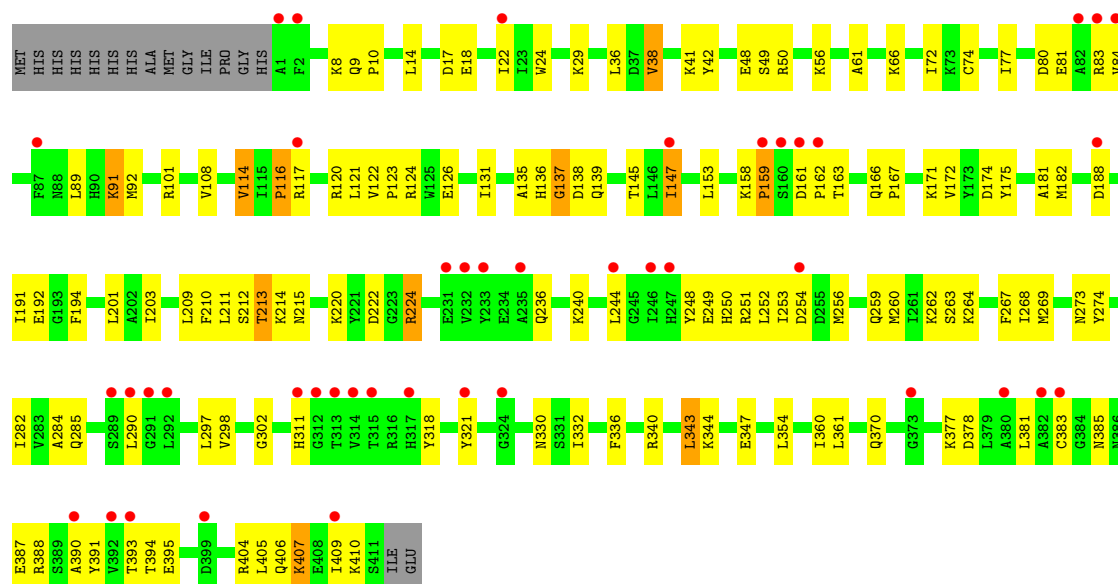


• Molecule 1: Isocitrate dehydrogenase [NADP]

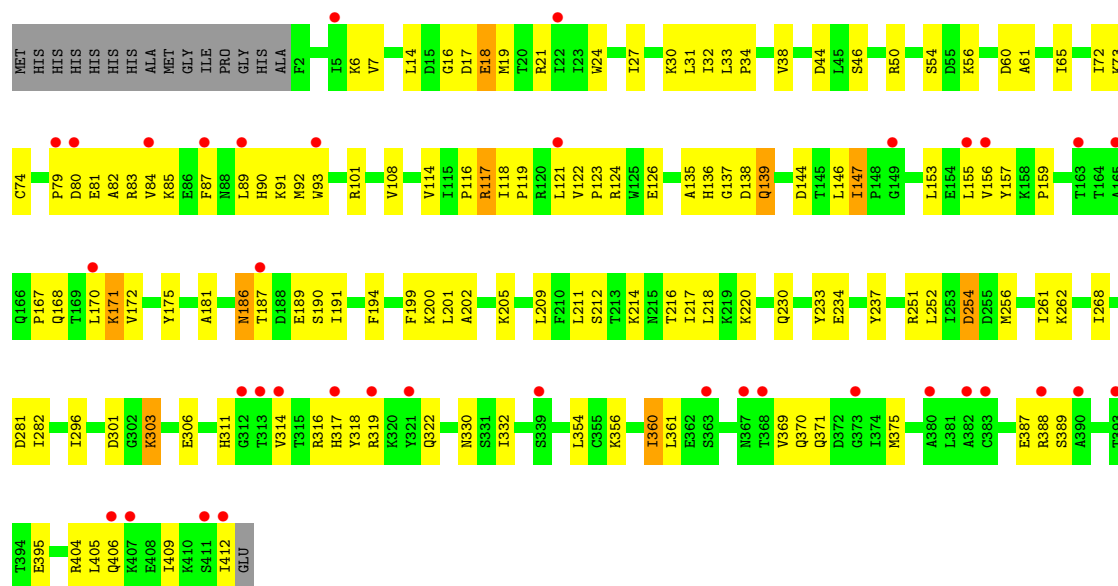


• Molecule 1: Isocitrate dehydrogenase [NADP]

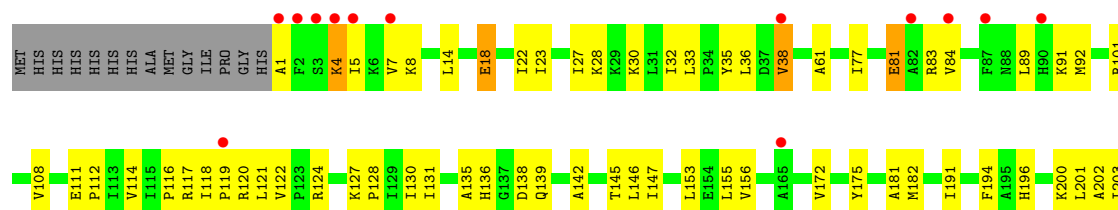


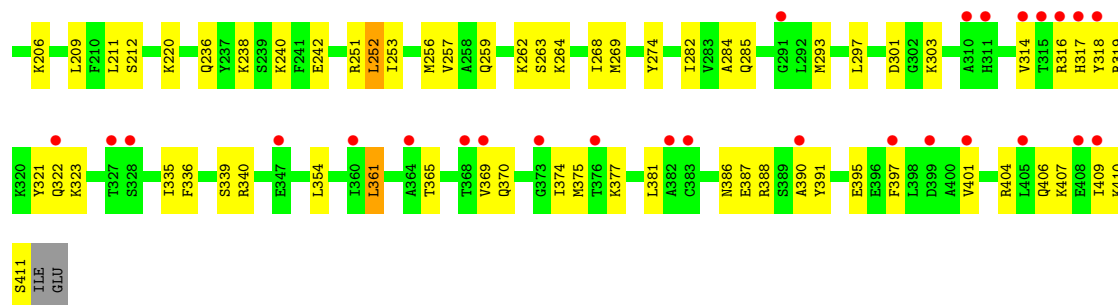


• Molecule 1: Isocitrate dehydrogenase [NADP]

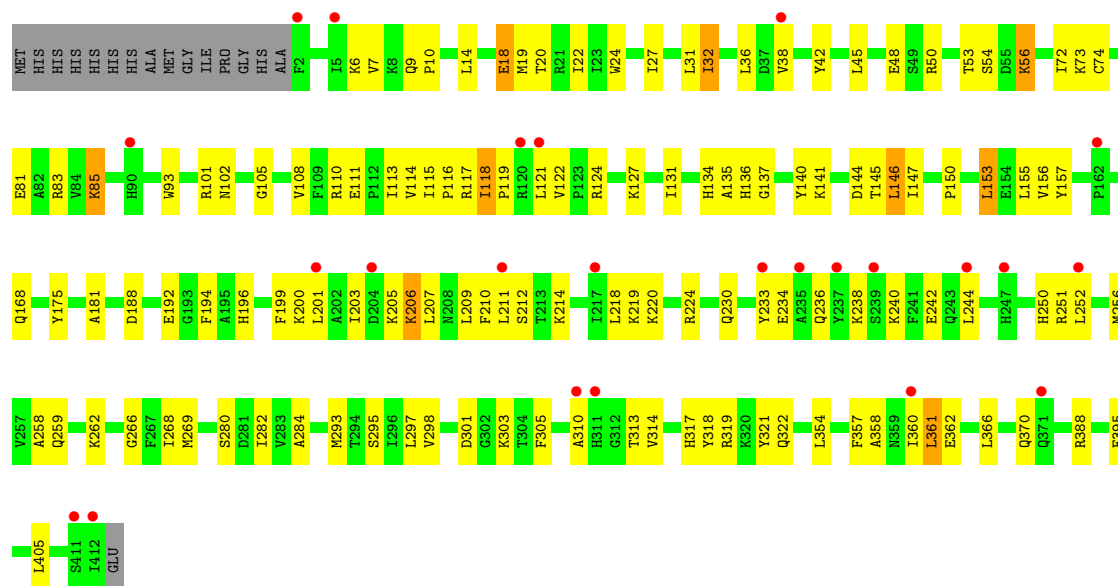


• Molecule 1: Isocitrate dehydrogenase [NADP]





● 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	74.90Å 98.48Å 190.60Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	43.65 – 2.10 43.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.65-2.10) 99.2 (43.65-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.08Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.247 0.208 , 0.206	Depositor DCC
R_{free} test set	8055 reflections (4.93%)	wwPDB-VP
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 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 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, 0.333 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	0.43	1/3319 (0.0%)	0.94	15/4477 (0.3%)
1	B	0.41	0/3316	1.03	22/4473 (0.5%)
1	C	0.35	0/3316	0.90	7/4473 (0.2%)
1	D	0.34	0/3319	0.87	11/4477 (0.2%)
1	E	0.33	0/3316	0.88	9/4473 (0.2%)
1	F	0.35	0/3319	0.90	13/4477 (0.3%)
All	All	0.37	1/19905 (0.0%)	0.92	77/26850 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	MET	SD-CE	-5.30	1.66	1.79

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	SER	N-CA-C	-26.45	68.87	109.86
1	B	3	SER	CB-CA-C	7.64	131.33	113.15
1	B	115	ILE	N-CA-C	-7.57	100.66	108.15
1	E	147	ILE	CA-C-N	7.49	127.03	119.24
1	E	147	ILE	C-N-CA	7.49	127.03	119.24
1	B	4	LYS	N-CA-CB	-7.16	98.34	111.37
1	D	114	VAL	N-CA-C	6.98	118.90	108.23
1	E	114	VAL	N-CA-C	6.85	118.68	108.54
1	C	122	VAL	CA-C-N	6.77	128.30	119.84
1	C	122	VAL	C-N-CA	6.77	128.30	119.84
1	A	136	HIS	N-CA-C	6.71	120.10	109.50
1	D	156	VAL	N-CA-C	6.68	117.53	108.17
1	C	114	VAL	N-CA-C	6.53	118.20	108.54
1	B	114	VAL	N-CA-C	6.50	118.17	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	VAL	CA-C-N	6.49	127.95	119.84
1	D	122	VAL	C-N-CA	6.49	127.95	119.84
1	B	122	VAL	CA-C-N	6.47	127.92	119.84
1	B	122	VAL	C-N-CA	6.47	127.92	119.84
1	D	136	HIS	N-CA-C	6.45	120.04	109.72
1	E	122	VAL	CA-C-N	6.43	127.87	119.84
1	E	122	VAL	C-N-CA	6.43	127.87	119.84
1	A	73	LYS	N-CA-C	6.25	119.09	108.90
1	F	118	ILE	N-CA-C	6.19	113.95	108.63
1	F	73	LYS	N-CA-C	6.17	118.96	108.90
1	D	147	ILE	CA-C-N	6.17	125.89	119.05
1	D	147	ILE	C-N-CA	6.17	125.89	119.05
1	A	122	VAL	CA-C-N	6.09	127.45	119.84
1	A	122	VAL	C-N-CA	6.09	127.45	119.84
1	A	156	VAL	N-CA-C	6.08	116.62	108.11
1	F	122	VAL	CA-C-N	6.06	127.41	119.84
1	F	122	VAL	C-N-CA	6.06	127.41	119.84
1	C	147	ILE	CA-C-N	6.03	125.25	118.97
1	C	147	ILE	C-N-CA	6.03	125.25	118.97
1	B	263	SER	N-CA-C	6.00	118.63	110.35
1	F	42	TYR	N-CA-C	5.94	119.20	109.76
1	F	156	VAL	N-CA-C	5.93	116.41	107.80
1	A	113	ILE	N-CA-C	-5.87	98.77	107.51
1	D	73	LYS	N-CA-C	5.86	119.02	109.59
1	F	32	ILE	N-CA-C	5.83	116.96	111.48
1	A	17	ASP	N-CA-C	5.81	119.04	109.85
1	D	17	ASP	N-CA-C	5.76	118.60	110.14
1	F	136	HIS	N-CA-C	5.75	118.92	109.72
1	D	139	GLN	N-CA-C	5.72	118.28	111.71
1	B	136	HIS	N-CA-C	5.71	122.97	110.80
1	B	161	ASP	CA-C-N	5.71	126.09	119.47
1	B	161	ASP	C-N-CA	5.71	126.09	119.47
1	B	113	ILE	N-CA-C	-5.71	99.01	107.51
1	F	137	GLY	N-CA-C	5.67	122.09	112.22
1	E	136	HIS	N-CA-C	5.61	118.69	109.72
1	F	113	ILE	N-CA-C	-5.60	99.17	107.51
1	B	176	LYS	N-CA-C	-5.51	105.91	113.30
1	C	17	ASP	N-CA-C	5.43	118.55	110.14
1	B	73	LYS	N-CA-C	5.40	118.20	109.40
1	E	156	VAL	N-CA-C	5.39	115.72	108.17
1	A	147	ILE	N-CA-C	-5.34	101.88	107.60
1	A	4	LYS	N-CA-C	5.32	117.94	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	GLY	N-CA-C	5.32	121.91	112.02
1	B	147	ILE	CA-C-N	5.28	124.78	119.19
1	B	147	ILE	C-N-CA	5.28	124.78	119.19
1	F	114	VAL	N-CA-C	5.27	116.29	108.23
1	A	42	TYR	N-CA-C	5.26	118.13	109.76
1	A	161	ASP	CA-C-N	5.24	125.55	119.47
1	A	161	ASP	C-N-CA	5.24	125.55	119.47
1	A	114	VAL	N-CA-C	5.23	116.11	108.58
1	A	176	LYS	N-CA-C	-5.19	105.82	113.61
1	B	37	ASP	N-CA-C	-5.18	98.87	107.99
1	C	42	TYR	N-CA-C	5.14	118.00	109.46
1	B	115	ILE	CA-C-N	5.13	126.26	119.84
1	B	115	ILE	C-N-CA	5.13	126.26	119.84
1	B	17	ASP	N-CA-C	5.11	117.93	109.85
1	F	147	ILE	CA-C-N	5.07	124.73	119.56
1	F	147	ILE	C-N-CA	5.07	124.73	119.56
1	E	252	LEU	N-CA-C	-5.05	102.80	110.28
1	B	38	VAL	N-CA-C	5.03	115.95	108.46
1	A	337	ALA	N-CA-C	-5.03	105.80	111.28
1	E	38	VAL	N-CA-C	5.02	115.19	108.17
1	B	410	LYS	N-CA-C	-5.01	107.30	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3256	0	3302	76	0
1	B	3253	0	3299	97	0
1	C	3253	0	3299	131	0
1	D	3256	0	3302	127	0
1	E	3253	0	3299	119	0
1	F	3256	0	3302	108	0
2	A	10	0	4	1	0
2	B	10	0	4	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	617	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 16.

All (617) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:MET:HE1	1:D:218:LEU:HD13	1.42	1.00
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:260:MET:SD	1:C:269:MET:HE1	2.15	0.86
1:E:182:MET:HE1	1:F:218:LEU:HD13	1.57	0.85
1:B:182:MET:HE2	1:B:184:MET:HE2	1.56	0.85
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:B:2:PHE:C	1:B:3:SER:O	2.02	0.82
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:A:260:MET:SD	1:A:269:MET:HE1	2.22	0.78
1:D:117:ARG:HH11	1:D:117:ARG:HB2	1.46	0.78
1:B:7:VAL:CG2	1:B:38:VAL:HG12	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:117:ARG:HD3	1:D:375:MET:HE1	1.67	0.76
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:E:153:LEU:HD12	1:E:172:VAL:HB	1.68	0.76
1:C:404:ARG:HA	1:C:407:LYS:HZ3	1.50	0.76
1:A:139:GLN:HG3	1:A:184:MET:HE1	1.66	0.75
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: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:C:81:GLU:CD	1:C:81:GLU:H	1.98	0.71
1:A:48:GLU:HG2	1:C:29:LYS:HD3	1.72	0.70
1:F:388:ARG:O	1:F:388:ARG:HD3	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:O	1:D:388:ARG:HD3	1.92	0.69
1:A:219:LYS:HE2	1:B:92:MET:HE2	1.74	0.69
1:B:388:ARG:O	1:B:388:ARG:HD3	1.93	0.69
1:E:369:VAL:HG13	1:E:375:MET:HB3	1.73	0.69
1:F:141:LYS:HE2	1:F:141:LYS:HA	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:E:395:GLU:H	1:E:395:GLU:CD	2.00	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:D:371:GLN:CD	1:D:404:ARG:HH22	2.03	0.67
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:C	1:B:32:ILE:HD12	2.20	0.67
1:C:213:THR:HG23	1:C:215:ASN:N	2.09	0.67
1:B:81:GLU:H	1:B:81:GLU:CD	2.03	0.66
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
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:249:GLU:CD	1:C:251:ARG:HE	2.04	0.65
1:C:123:PRO:HG2	1:D:123:PRO:HG2	1.79	0.65
1:B:388:ARG:HD3	1:B:388:ARG:C	2.21	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:C:91:LYS:HG2	1:C:92:MET:N	2.11	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:D:369:VAL:HG13	1:D:375:MET:HE2	1.81	0.63
1:E:301:ASP:OD1	1:E:303:LYS:HG2	1.97	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:360:ILE:C	1:D:360:ILE:HD12	2.23	0.62
1:F:297:LEU:HD23	1:F:298:VAL:N	2.14	0.62
1:D:356:LYS:HZ1	1:D:412:ILE:HA	1.65	0.62
1:A:131:ILE:CD1	1:A:269:MET:HE3	2.30	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:D:388:ARG:HD3	1:D:388:ARG:C	2.25	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:E:14:LEU:CD2	1:E:61:ALA:HB1	2.31	0.61
1:B:3:SER:C	3:B:2175:HOH:O	2.43	0.61
1:D:153:LEU:HD12	1:D:172:VAL:CB	2.30	0.61
1:D:387:GLU:OE2	1:D:389:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:VAL:HG23	1:E:89:LEU:HB2	1.83	0.61
1:E:284:ALA:HB2	1:E:293:MET:HE2	1.81	0.61
1:F:157:TYR:HB3	1:F:168:GLN:HB2	1.81	0.61
1:C:251:ARG:HH12	1:C:259:GLN:CD	2.07	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:HB2	1:D:171:LYS:NZ	2.16	0.60
1:F:48:GLU:HG3	3:F:2015:HOH:O	2.02	0.60
1:B:318:TYR:O	1:B:322:GLN:HG2	2.02	0.60
1:C:201:LEU:HD12	1:C:268:ILE:CD1	2.32	0.60
1:C:252:LEU:HD11	1:C:254:ASP:OD2	2.01	0.60
1:E:388:ARG:O	1:E:388:ARG:HD3	2.01	0.60
1:F:201:LEU:HD13	1:F:205:LYS:HG3	1.84	0.60
1:B:393:THR:HG22	1:B:396:GLU:CD	2.27	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:388:ARG:O	1:C:388:ARG:HD3	2.01	0.59
1:F:238:LYS:O	1:F:242:GLU:HG3	2.03	0.59
1:F:256:MET:HG3	1:F:269:MET:HE3	1.83	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:B:297:LEU:C	1:B:297:LEU:HD23	2.28	0.59
1:B:136:HIS:C	3:B:2275:HOH:O	2.42	0.58
1:A:240:LYS:HG2	3:A:2342:HOH:O	2.03	0.58
3:A:2122:HOH:O	1:B:92:MET:HE1	2.02	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:117:ARG:HH11	1:D:117:ARG:CB	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:B:326:GLU:CD	1:B:388:ARG:HH21	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:LEU:C	1:C:297:LEU:HD23	2.29	0.57
1:C:201:LEU:HD12	1:C:268:ILE:HD13	1.86	0.57
1:F:388:ARG:HD3	1:F:388:ARG:C	2.29	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:B:256:MET:HG3	1:B:269:MET:HE3	1.85	0.57
1:C:406:GLN:O	1:C:410:LYS:HG3	2.05	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:D:31:LEU:C	1:D:32:ILE:HD12	2.30	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:F:210:PHE:CD2	1:F:251:ARG:HD2	2.39	0.57
1:B:1:ALA:C	1:B:3:SER:O	2.47	0.56
1:C:209:LEU:HD12	1:C:248:TYR:CD1	2.41	0.56
1:C:404:ARG:HG2	1:C:404:ARG:HH11	1.71	0.56
1:D:90:HIS:O	1:D:91:LYS:HB2	2.05	0.56
1:D:124:ARG:O	1:D:126:GLU:HG3	2.04	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:C:182:MET:HE1	1:D:218:LEU:CD1	2.27	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:GLU:CD	1:D:395:GLU:H	2.15	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:HH11	1:B:319:ARG:HB2	1.72	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:OE1	1:F:395:GLU:N	2.37	0.54
1:B:213:THR:HG21	1:B:215:ASN:HB3	1.88	0.54
1:B:32:ILE:HD12	1:B:32:ILE:N	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: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:F:31:LEU:C	1:F:32:ILE:HD12	2.33	0.53
1:F:297:LEU:HD23	1:F:297:LEU:C	2.34	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:HD12	1:D:32:ILE:N	2.24	0.53
1:A:282:ILE:HD13	1:B:282:ILE:HD13	1.91	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:D:214:LYS:HG3	1:D:217:ILE:HD13	1.90	0.52
1:D:319:ARG:HB3	1:D:319:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:ASP:CG	1:F:303:LYS:HG2	2.34	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:E:256:MET:HG3	1:E:269:MET:HE3	1.92	0.52
1:A:377:LYS:O	1:A:381:LEU:HD13	2.10	0.52
1:C:297:LEU:HD23	1:C:298:VAL:N	2.25	0.52
1:E:297:LEU:HD13	1:E:297:LEU:C	2.35	0.52
1:B:256:MET:CG	1:B:269:MET:HE3	2.39	0.52
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.75	0.52
1:F:83:ARG:HB2	1:F:83:ARG:NH1	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
1:E:238:LYS:O	1:E:242:GLU:HG3	2.10	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:7:VAL:CG2	1:F:38:VAL:HG22	2.40	0.51
1:F:318:TYR:O	1:F:322:GLN:HG3	2.11	0.51
1:B:213:THR:HG22	1:B:250:HIS:NE2	2.25	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:116:PRO:HG2	1:E:370:GLN:CD	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:HG22	1:A:32:ILE:HD13	1.94	0.50
1:E:22:ILE:HD13	1:E:321:TYR:CE2	2.46	0.50
1:E:316:ARG:HG3	1:E:317:HIS:N	2.27	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:9:GLN:HG3	1:A:10:PRO:HD2	1.94	0.49
1:A:10:PRO:HG2	1:A:68:TYR:CD2	2.47	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: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:C:131:ILE:HD11	1:C:269:MET:HE3	1.95	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:B:356:LYS:HB3	1:B:356:LYS:HZ2	1.74	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:A:182:MET:HE2	1:A:184:MET:CE	2.44	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:A:131:ILE:HD13	1:A:269:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:ARG:NE	3:C:2143:HOH:O	2.47	0.48
1:D:262:LYS:O	1:D:262:LYS:HG2	2.13	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:HD12	1:E:32:ILE:N	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
1:C:211:LEU:HD13	1:C:211:LEU:C	2.39	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:D:406:GLN:O	1:D:409:ILE:HG22	2.14	0.48
1:E:182:MET:HE1	1:F:218:LEU:CD1	2.39	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:E:319:ARG:NH1	1:E:319:ARG:HB3	2.29	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:161:ASP:C	1:C:163:THR:H	2.21	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:C:254:ASP:HB3	1:D:281:ASP:OD1	2.15	0.47
1:D:319:ARG:HB3	1:D:319:ARG:CZ	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: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:D:171:LYS:HB2	1:D:171:LYS:HZ2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:GLU:C	1:E:84:VAL:HG12	2.40	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:F:360:ILE:HD12	1:F:360:ILE:C	2.40	0.47
1:A:31:LEU:C	1:A:32:ILE:HD12	2.39	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:C:282:ILE:HD13	1:D:282:ILE:HD13	1.97	0.46
1:D:170:LEU:N	1:D:170:LEU:HD22	2.30	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:HD12	1:D:89:LEU:N	2.31	0.46
1:F:201:LEU:CD1	1:F:205:LYS:HG3	2.44	0.46
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:129:ILE:CG2	1:A:269:MET:HE2	2.45	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:HB3	1:E:124:ARG:HH11	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:29:LYS:HE3	1:C:49:SER:HA	1.96	0.46
1:A:109:PHE:CE1	1:A:201:LEU:HD12	2.50	0.46
1:F:24:TRP:CD2	1:F:74:CYS:HB2	2.51	0.46
1:C:159:PRO:C	1:C:161:ASP:H	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:HG3	3:A:2248:HOH:O	2.15	0.45
1:C:388:ARG:HD3	1:C:388:ARG:C	2.41	0.45
1:E:153:LEU:HD12	1:E:172:VAL:CB	2.43	0.45
1:A:139:GLN:HG3	1:A:184:MET:CE	2.41	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: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:F:211:LEU:HD12	1:F:250:HIS:CD2	2.51	0.45
1:D:395:GLU:CD	1:D:395:GLU:N	2.75	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:C:161:ASP:O	1:C:163:THR:N	2.47	0.45
1:C:159:PRO:C	1:C:161:ASP:N	2.74	0.45
1:F:199:PHE:CZ	1:F:233:TYR:HB2	2.52	0.45
1:F:256:MET:HE3	1:F:256:MET:O	2.17	0.45
1:F:256:MET:CG	1:F:269:MET:HE3	2.47	0.45
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:32:ILE:HD12	1:F:32:ILE:N	2.32	0.45
1:F:205:LYS:O	1:F:207:LEU:HG	2.17	0.45
1:A:131:ILE:HD11	1:A:269:MET:HE3	1.97	0.44
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:F:301:ASP:OD1	1:F:303:LYS:HG2	2.17	0.44
1:E:124:ARG:HH12	1:E:263:SER:C	2.25	0.44
1:E:196:HIS:O	1:E:200:LYS:HG3	2.17	0.44
1:A:14:LEU:HD22	1:A:61:ALA:HB1	1.98	0.44
1:A:24:TRP:CD2	1:A:74:CYS:HB2	2.52	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:D:356:LYS:HZ3	1:D:412:ILE:HG23	1.82	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:B:372:ASP:CG	1:B:404:ARG:HH21	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:ARG:HD2	3:F:2007:HOH:O	2.17	0.44
1:F:295:SER:CB	1:F:310:ALA:HB2	2.47	0.44
1:B:182:MET:CE	1:B:184:MET:HE2	2.37	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:14:LEU:HD21	1:E:61:ALA:HB1	2.00	0.43
1:E:111:GLU:HB2	1:E:112:PRO:HD2	2.00	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: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:OE1	1:F:81:GLU:HA	2.19	0.43
1:A:224:ARG:NH2	1:A:228:ILE:HD11	2.33	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:120:ARG:HG2	1:A:120:ARG:NH1	2.27	0.43
1:B:14:LEU:HD22	1:B:61:ALA:HB1	2.01	0.43
1:B:18:GLU:HB3	1:B:318:TYR:CG	2.54	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: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: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:C:330:ASN:HB2	1:C:378:ASP:OD2	2.18	0.43
1:F:22:ILE:HD13	1:F:321:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:ARG:N	1:A:370:GLN:HE22	2.03	0.42
1:A:214:LYS:HD2	1:A:252:LEU:HD11	2.01	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:213:THR:OG1	1:C:222:ASP:HB3	2.18	0.42
1:C:213:THR:HG21	1:C:215:ASN:HB3	2.00	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:NZ	1:F:262:LYS:HB3	2.33	0.42
1:F:284:ALA:HB2	1:F:293:MET:HE2	2.01	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: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: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: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:C:388:ARG:C	1:C:390:ALA:H	2.25	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: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:HB3	1:C:124:ARG:NH1	2.35	0.42
1:D:21:ARG:HH22	1:D:44:ASP:CG	2.27	0.42
1:D:388:ARG:C	1:D:388:ARG:CD	2.93	0.42
1:C:209:LEU:HD13	1:C:210:PHE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LEU:HD23	1:D:405:LEU:C	2.45	0.42
1:E:282:ILE:HD13	1:F:282:ILE:HD13	2.01	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:A:404:ARG:NH2	3:A:2170:HOH:O	2.52	0.42
1:B:297:LEU:C	1:B:297:LEU:CD2	2.93	0.42
1:F:211:LEU:C	1:F:211:LEU:HD13	2.45	0.42
1:B:314:VAL:HG12	1:B:316:ARG:HG2	2.02	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: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:209:LEU:HD13	1:C:209:LEU:C	2.45	0.41
1:C:336:PHE:O	1:C:340:ARG:HG2	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:D:153:LEU:HD13	1:D:153:LEU:C	2.45	0.41
1:E:274:TYR:HE1	1:F:214:LYS:HG3	1.86	0.41
1:A:31:LEU:HB2	1:A:32:ILE:HD12	2.01	0.41
1:A:120:ARG:HG3	3:A:2389:HOH:O	2.20	0.41
1:C:24:TRP:CH2	1:C:72:ILE:HG22	2.55	0.41
1:C:50:ARG:HD2	3:C:2005:HOH:O	2.20	0.41
1:C:267:PHE:HE1	1:C:269:MET:HE2	1.85	0.41
1:C:387:GLU:HG2	1:C:390:ALA:CB	2.49	0.41
1:D:116:PRO:HB2	1:D:370:GLN:OE1	2.20	0.41
1:D:214:LYS:HE3	1:D:254:ASP:OD1	2.20	0.41
1:E:365:THR:HA	1:E:401:VAL:HG13	2.03	0.41
1:F:32:ILE:HG23	1:F:36:LEU:HD12	2.02	0.41
1:F:224:ARG:HD2	3:F:2035:HOH:O	2.20	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: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: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:D:83:ARG:C	1:D:85:LYS:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:185:TYR:CD1	1:A:185:TYR:C	2.98	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:E:30:LYS:NZ	1:E:30:LYS:HB3	2.36	0.41
1:E:92:MET:HE2	1:F:219:LYS:CE	2.50	0.41
1:E:319:ARG:NH1	1:E:319:ARG:CB	2.82	0.41
1:E:321:TYR:C	1:E:323:LYS:H	2.28	0.41
1:F:118:ILE:HA	1:F:119:PRO:HD3	1.87	0.41
1:F:297:LEU:C	1:F:297:LEU:CD2	2.93	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:79:PRO:HG2	1:D:93:TRP:O	2.20	0.41
1:D:138:ASP:HB3	1:D:139:GLN:OE1	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:D:296:ILE:O	1:D:296:ILE:HG23	2.20	0.41
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:E:7:VAL:CB	1:E:38:VAL:HG12	2.51	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:153:LEU:CD1	1:E:172:VAL:HB	2.44	0.41
1:E:369:VAL:HG22	1:E:374:ILE:O	2.20	0.41
1:F:140:TYR:CD1	1:F:140:TYR:N	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:CD1	1:B:140:TYR:N	2.90	0.40
1:C:8:LYS:NZ	3:C:2135:HOH:O	2.53	0.40
1:C:114:VAL:HG12	1:C:116:PRO:HD3	2.02	0.40
1:C:153:LEU:C	1:C:153:LEU:HD13	2.47	0.40
1:C:212:SER:HB3	1:C:253:ILE:HA	2.04	0.40
1:D:32:ILE:N	1:D:32:ILE:CD1	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:20:THR:OG1	1:B:313:THR:HB	2.21	0.40
1:C:121:LEU:C	1:C:123:PRO:HD3	2.46	0.40
1:C:201:LEU:HD12	1:C:268:ILE:HD11	2.04	0.40
1:D:80:ASP:O	1:D:81:GLU:C	2.65	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
1:D:117:ARG:CD	1:D:375:MET:HE1	2.44	0.40
1:E:4:LYS:HA	1:E:35:TYR:O	2.21	0.40
1:E:146:LEU:HD12	1:F:220:LYS:HB3	2.02	0.40
1:E:319:ARG:CB	1:E:319:ARG:HH11	2.34	0.40
1:E:335:ILE:CG2	1:E:361:LEU:HD22	2.52	0.40
1:F:14:LEU:HD13	1:F:45:LEU:HD11	2.03	0.40
1:A:121:LEU:CD1	1:A:285:GLN:HE21	2.34	0.40
1:C:404:ARG:HA	1:C:407:LYS:NZ	2.26	0.40
1:D:65:ILE:HD13	1:D:306:GLU:HG3	2.02	0.40
1:E:256:MET:CG	1:E:269:MET:HE3	2.50	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%)	24	22
1	C	409/427 (96%)	378 (92%)	25 (6%)	6 (2%)	8	4
1	D	409/427 (96%)	384 (94%)	23 (6%)	2 (0%)	24	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	409/427 (96%)	382 (93%)	23 (6%)	4 (1%)	12	9
1	F	409/427 (96%)	394 (96%)	13 (3%)	2 (0%)	24	22
All	All	2454/2562 (96%)	2325 (95%)	113 (5%)	16 (1%)	18	15

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%)	339 (96%)	16 (4%)	24	25
1	B	354/367 (96%)	341 (96%)	13 (4%)	30	33
1	C	354/367 (96%)	343 (97%)	11 (3%)	35	39
1	D	355/367 (97%)	344 (97%)	11 (3%)	35	39
1	E	354/367 (96%)	347 (98%)	7 (2%)	48	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	355/367 (97%)	343 (97%)	12 (3%)	32	35
All	All	2127/2202 (97%)	2057 (97%)	70 (3%)	33	37

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	38	VAL
1	A	116	PRO
1	A	146	LEU
1	A	153	LEU
1	A	155	LEU
1	A	171	LYS
1	A	201	LEU
1	A	209	LEU
1	A	211	LEU
1	A	303	LYS
1	A	354	LEU
1	A	361	LEU
1	A	388	ARG
1	A	405	LEU
1	A	409	ILE
1	B	9	GLN
1	B	48	GLU
1	B	139	GLN
1	B	153	LEU
1	B	155	LEU
1	B	201	LEU
1	B	209	LEU
1	B	211	LEU
1	B	213	THR
1	B	252	LEU
1	B	354	LEU
1	B	361	LEU
1	B	405	LEU
1	C	9	GLN
1	C	38	VAL
1	C	48	GLU
1	C	56	LYS
1	C	91	LYS
1	C	213	THR
1	C	224	ARG

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Mol	Chain	Res	Type
1	C	343	LEU
1	C	354	LEU
1	C	361	LEU
1	C	407	LYS
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	360	ILE
1	D	361	LEU
1	E	81	GLU
1	E	206	LYS
1	E	209	LEU
1	E	211	LEU
1	E	252	LEU
1	E	354	LEU
1	E	361	LEU
1	F	6	LYS
1	F	56	LYS
1	F	85	LYS
1	F	116	PRO
1	F	146	LEU
1	F	153	LEU
1	F	155	LEU
1	F	206	LYS
1	F	209	LEU
1	F	354	LEU
1	F	361	LEU
1	F	405	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	236	GLN
1	A	243	GLN
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	285	GLN
1	A	317	HIS
1	A	350	ASN
1	A	370	GLN
1	A	406	GLN
1	B	236	GLN
1	B	279	GLN
1	B	311	HIS
1	B	370	GLN
1	B	385	ASN
1	B	406	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	243	GLN
1	D	279	GLN
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	279	GLN
1	E	322	GLN
1	E	367	ASN
1	E	370	GLN
1	F	88	ASN
1	F	102	ASN
1	F	168	GLN
1	F	230	GLN
1	F	259	GLN
1	F	279	GLN
1	F	317	HIS
1	F	322	GLN
1	F	370	GLN

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Mol	Chain	Res	Type
1	F	371	GLN
1	F	386	ASN
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 oligosaccharides 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	B	2002	-	9,9,9	1.28	1 (11%)	11,11,11	1.50	2 (18%)
2	AKG	E	2005	-	9,9,9	1.26	1 (11%)	11,11,11	1.51	2 (18%)
2	AKG	C	2003	-	9,9,9	1.28	1 (11%)	11,11,11	1.48	2 (18%)
2	AKG	D	2004	-	9,9,9	1.27	1 (11%)	11,11,11	1.50	2 (18%)
2	AKG	F	2006	-	9,9,9	1.27	1 (11%)	11,11,11	1.51	2 (18%)
2	AKG	A	2001	-	9,9,9	1.29	1 (11%)	11,11,11	1.50	2 (18%)

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	B	2002	-	-	4/9/9/9	-
2	AKG	E	2005	-	-	1/9/9/9	-
2	AKG	C	2003	-	-	2/9/9/9	-
2	AKG	D	2004	-	-	1/9/9/9	-
2	AKG	F	2006	-	-	3/9/9/9	-
2	AKG	A	2001	-	-	3/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	AKG	C3-C2	2.18	1.53	1.51
2	C	2003	AKG	C3-C2	2.15	1.53	1.51
2	D	2004	AKG	C3-C2	2.09	1.53	1.51
2	B	2002	AKG	C3-C2	2.08	1.53	1.51
2	F	2006	AKG	C3-C2	2.07	1.53	1.51
2	E	2005	AKG	C3-C2	2.00	1.53	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2006	AKG	O1-C1-C2	-3.08	117.98	121.81
2	D	2004	AKG	O1-C1-C2	-3.06	118.01	121.81
2	A	2001	AKG	O1-C1-C2	-3.04	118.03	121.81
2	C	2003	AKG	O1-C1-C2	-3.04	118.03	121.81
2	E	2005	AKG	O1-C1-C2	-3.03	118.05	121.81
2	B	2002	AKG	O1-C1-C2	-3.00	118.08	121.81
2	E	2005	AKG	C3-C2-C1	2.45	120.03	115.86
2	C	2003	AKG	C3-C2-C1	2.38	119.90	115.86
2	D	2004	AKG	C3-C2-C1	2.33	119.82	115.86
2	B	2002	AKG	C3-C2-C1	2.32	119.81	115.86
2	A	2001	AKG	C3-C2-C1	2.30	119.76	115.86
2	F	2006	AKG	C3-C2-C1	2.23	119.65	115.86

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	AKG	C1-C2-C3-C4
2	B	2002	AKG	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	C	2003	AKG	C1-C2-C3-C4
2	D	2004	AKG	C1-C2-C3-C4
2	E	2005	AKG	C1-C2-C3-C4
2	F	2006	AKG	C1-C2-C3-C4
2	B	2002	AKG	O5-C2-C3-C4
2	F	2006	AKG	C3-C4-C5-O4
2	F	2006	AKG	C3-C4-C5-O3
2	B	2002	AKG	C3-C4-C5-O4
2	B	2002	AKG	C3-C4-C5-O3
2	A	2001	AKG	C3-C4-C5-O4
2	C	2003	AKG	O5-C2-C3-C4
2	A	2001	AKG	C3-C4-C5-O3

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	AKG	3	0
2	E	2005	AKG	1	0
2	C	2003	AKG	1	0
2	D	2004	AKG	3	0
2	F	2006	AKG	2	0
2	A	2001	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, 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%)	0.07	8 (1%) 66 69	23, 34, 55, 89	0
1	B	411/427 (96%)	0.24	17 (4%) 41 43	21, 36, 65, 103	0
1	C	411/427 (96%)	0.78	43 (10%) 11 12	31, 48, 86, 103	0
1	D	411/427 (96%)	0.75	37 (9%) 15 16	34, 49, 89, 103	0
1	E	411/427 (96%)	0.93	40 (9%) 13 14	36, 53, 101, 128	0
1	F	411/427 (96%)	0.59	24 (5%) 29 30	31, 46, 73, 108	0
All	All	2466/2562 (96%)	0.56	169 (6%) 23 24	21, 45, 83, 128	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	PHE	5.7
1	C	291	GLY	5.5
1	F	412	ILE	5.3
1	E	1	ALA	5.3
1	C	313	THR	4.5
1	D	87	PHE	4.5
1	E	405	LEU	4.2
1	B	1	ALA	4.1
1	B	3	SER	4.1
1	E	383	CYS	4.0
1	E	368	THR	4.0
1	C	1	ALA	4.0
1	C	314	VAL	4.0
1	E	327	THR	3.9
1	B	409	ILE	3.8
1	C	2	PHE	3.7
1	B	312	GLY	3.6
1	D	412	ILE	3.6
1	D	407	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	390	ALA	3.6
1	D	89	LEU	3.6
1	C	290	LEU	3.5
1	B	411	SER	3.5
1	C	160	SER	3.5
1	D	411	SER	3.5
1	F	360	ILE	3.4
1	E	328	SER	3.4
1	D	165	ALA	3.4
1	E	90	HIS	3.4
1	C	87	PHE	3.3
1	E	311	HIS	3.2
1	C	161	ASP	3.2
1	D	380	ALA	3.2
1	D	80	ASP	3.2
1	C	117	ARG	3.2
1	D	321	TYR	3.1
1	D	314	VAL	3.1
1	D	79	PRO	3.1
1	F	2	PHE	3.0
1	F	204	ASP	3.0
1	C	159	PRO	2.9
1	F	371	GLN	2.9
1	D	383	CYS	2.9
1	F	311	HIS	2.9
1	E	4	LYS	2.9
1	E	314	VAL	2.8
1	D	313	THR	2.8
1	C	147	ILE	2.8
1	E	5	ILE	2.8
1	F	90	HIS	2.8
1	E	318	TYR	2.8
1	E	2	PHE	2.8
1	B	2	PHE	2.7
1	F	237	TYR	2.7
1	D	319	ARG	2.7
1	D	406	GLN	2.7
1	A	90	HIS	2.7
1	B	311	HIS	2.7
1	C	399	ASP	2.7
1	F	310	ALA	2.7
1	D	363	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	411	SER	2.7
1	C	83	ARG	2.7
1	C	317	HIS	2.7
1	A	412	ILE	2.6
1	A	311	HIS	2.6
1	E	82	ALA	2.6
1	C	246	ILE	2.6
1	C	392	VAL	2.6
1	E	409	ILE	2.6
1	C	383	CYS	2.6
1	D	317	HIS	2.6
1	F	247	HIS	2.6
1	E	376	THR	2.6
1	B	82	ALA	2.5
1	C	315	THR	2.5
1	C	382	ALA	2.5
1	B	87	PHE	2.5
1	D	187	THR	2.5
1	E	408	GLU	2.5
1	F	244	LEU	2.5
1	D	5	ILE	2.5
1	C	393	THR	2.5
1	D	170	LEU	2.5
1	C	373	GLY	2.5
1	D	84	VAL	2.4
1	E	84	VAL	2.4
1	E	369	VAL	2.4
1	E	399	ASP	2.4
1	C	162	PRO	2.4
1	B	410	LYS	2.4
1	C	244	LEU	2.4
1	D	367	ASN	2.4
1	E	322	GLN	2.4
1	E	364	ALA	2.4
1	F	235	ALA	2.4
1	C	292	LEU	2.4
1	C	231	GLU	2.4
1	E	360	ILE	2.4
1	B	83	ARG	2.4
1	C	233	TYR	2.3
1	E	397	PHE	2.3
1	F	5	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	368	THR	2.3
1	B	321	TYR	2.3
1	D	149	GLY	2.3
1	A	228	ILE	2.3
1	E	401	VAL	2.3
1	F	38	VAL	2.3
1	D	390	ALA	2.3
1	E	390	ALA	2.3
1	D	373	GLY	2.3
1	A	126	GLU	2.3
1	A	409	ILE	2.3
1	E	119	PRO	2.3
1	B	393	THR	2.2
1	C	84	VAL	2.2
1	F	162	PRO	2.2
1	F	120	ARG	2.2
1	E	310	ALA	2.2
1	D	121	LEU	2.2
1	C	232	VAL	2.2
1	F	252	LEU	2.2
1	C	311	HIS	2.2
1	D	93	TRP	2.2
1	C	22	ILE	2.2
1	C	409	ILE	2.2
1	B	314	VAL	2.2
1	D	312	GLY	2.2
1	D	155	LEU	2.2
1	D	388	ARG	2.2
1	E	316	ARG	2.2
1	A	171	LYS	2.2
1	B	315	THR	2.2
1	E	87	PHE	2.1
1	D	156	VAL	2.1
1	E	38	VAL	2.1
1	E	382	ALA	2.1
1	C	289	SER	2.1
1	F	239	SER	2.1
1	B	38	VAL	2.1
1	E	373	GLY	2.1
1	D	382	ALA	2.1
1	E	165	ALA	2.1
1	D	339	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	121	LEU	2.1
1	E	315	THR	2.1
1	E	291	GLY	2.1
1	C	380	ALA	2.1
1	F	211	LEU	2.1
1	B	399	ASP	2.1
1	C	188	ASP	2.1
1	C	82	ALA	2.1
1	F	201	LEU	2.0
1	E	317	HIS	2.0
1	C	324	GLY	2.0
1	D	22	ILE	2.0
1	F	217	ILE	2.0
1	E	7	VAL	2.0
1	E	347	GLU	2.0
1	E	3	SER	2.0
1	C	235	ALA	2.0
1	C	254	ASP	2.0
1	C	247	HIS	2.0
1	D	163	THR	2.0
1	D	393	THR	2.0
1	C	312	GLY	2.0
1	C	321	TYR	2.0
1	F	233	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AKG	C	2003	10/10	0.65	0.23	75,77,80,80	10
2	AKG	D	2004	10/10	0.66	0.18	87,88,91,91	0
2	AKG	B	2002	10/10	0.68	0.30	76,77,80,80	10
2	AKG	E	2005	10/10	0.68	0.23	83,84,87,87	10
2	AKG	F	2006	10/10	0.75	0.25	80,82,85,87	9
2	AKG	A	2001	10/10	0.76	0.20	72,74,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.