



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:15 pm BST

PDB ID : 2QFX
Title : Crystal structure of *Saccharomyces cerevesiae* mitochondrial NADP(+)-dependent isocitrate dehydrogenase in complex with NADPH, α -ketoglutarate and $\text{Ca}(2+)$
Authors : Peng, Y.J.; Ding, J.P.
Deposited on : 2007-06-28
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

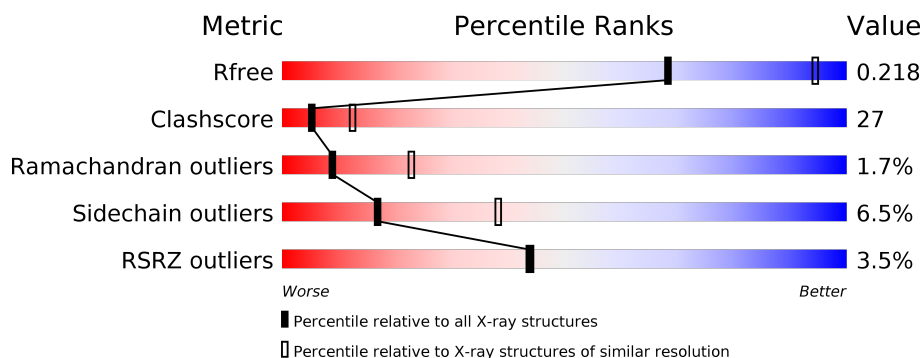
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>39%</div> <div>5%</div> </div> </div>
1	B	427	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>39%</div> <div>5%</div> </div> </div>
1	C	427	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>39%</div> <div></div> </div> </div>
1	D	427	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div></div> </div> </div>
1	E	427	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div></div> </div> </div>
1	F	427	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div></div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AKG	A	1102	-	-	X	-
4	AKG	B	1202	-	-	X	-
4	AKG	C	1302	-	-	X	-
4	AKG	D	1402	-	-	X	-
4	AKG	E	1502	-	-	X	-
4	AKG	F	1602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20069 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	410	Total	C	N	O	S	0	0	0
			3248	2070	550	616	12			
1	B	410	Total	C	N	O	S	0	0	0
			3248	2070	550	616	12			
1	C	410	Total	C	N	O	S	0	0	0
			3248	2070	550	616	12			
1	D	410	Total	C	N	O	S	0	0	0
			3248	2070	550	616	12			
1	E	410	Total	C	N	O	S	0	0	0
			3248	2070	550	616	12			
1	F	410	Total	C	N	O	S	0	0	0
			3248	2070	550	616	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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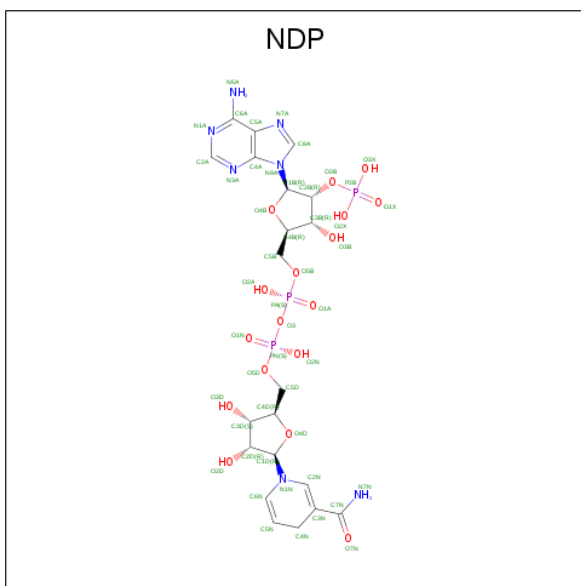
Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP P21954
E	-9	HIS	-	EXPRESSION TAG	UNP P21954
E	-8	HIS	-	EXPRESSION TAG	UNP P21954
E	-7	HIS	-	EXPRESSION TAG	UNP P21954
E	-6	ALA	-	EXPRESSION TAG	UNP P21954
E	-5	MET	-	EXPRESSION TAG	UNP P21954
E	-4	GLY	-	EXPRESSION TAG	UNP 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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

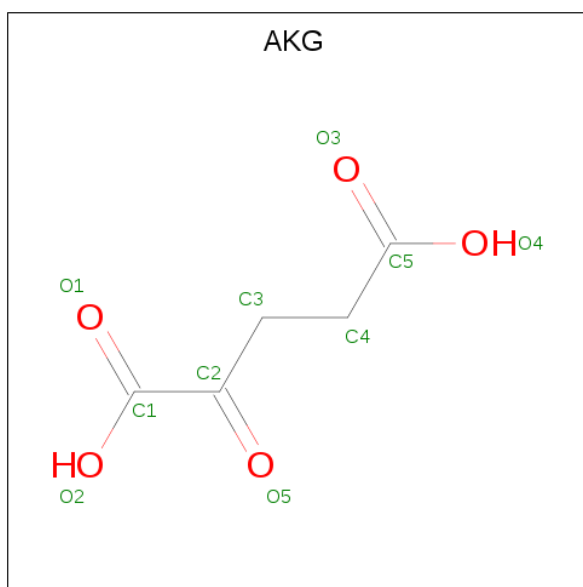
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



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

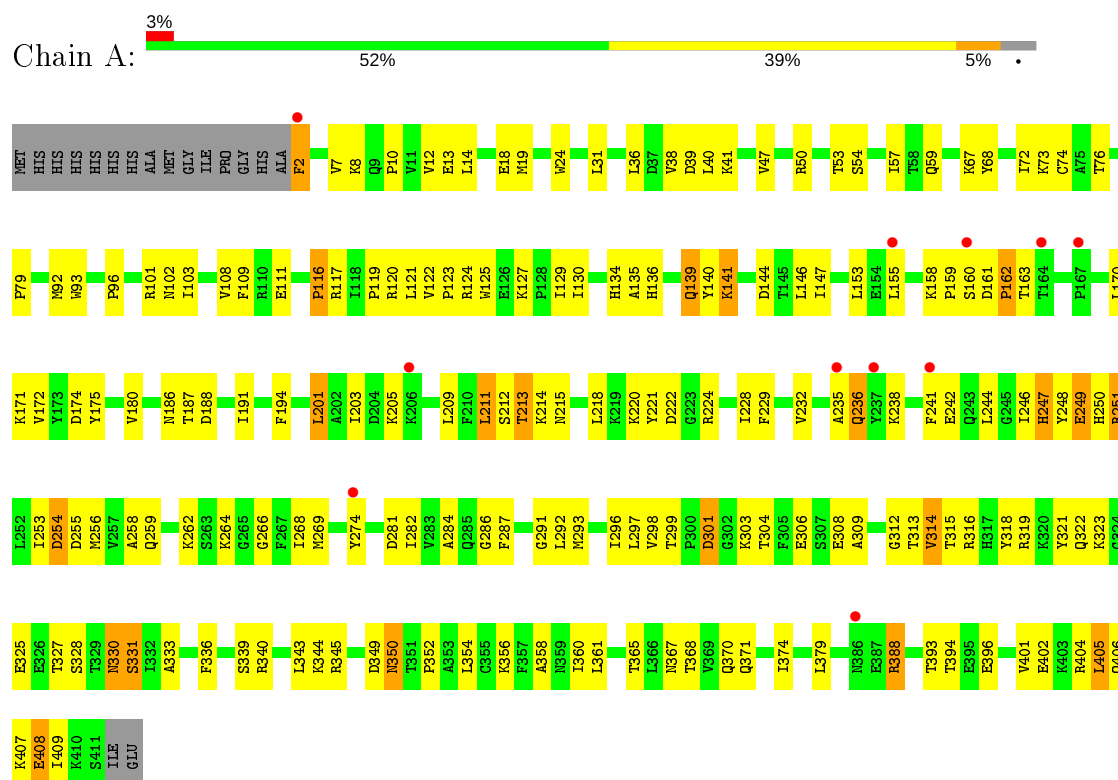
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	22	Total	O	0	0
			22	22		
5	C	47	Total	O	0	0
			47	47		
5	D	49	Total	O	0	0
			49	49		
5	E	30	Total	O	0	0
			30	30		
5	F	53	Total	O	0	0
			53	53		

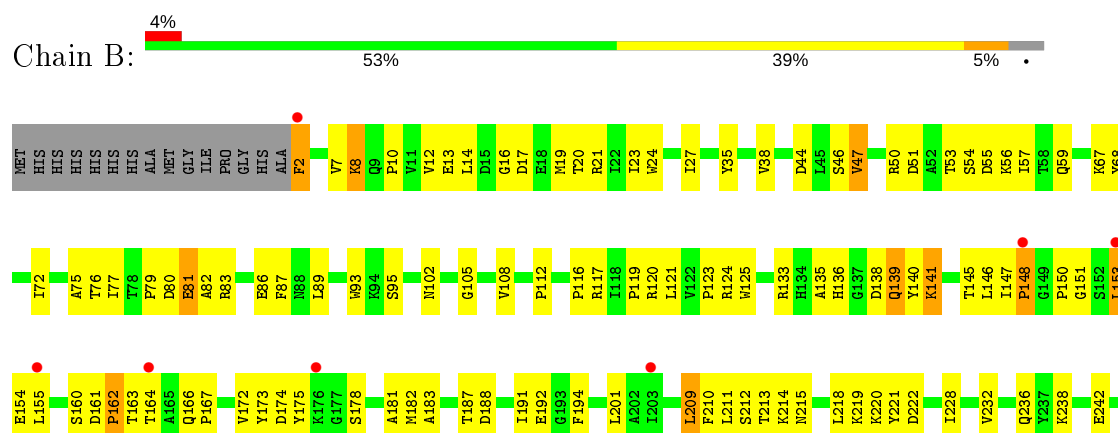
3 Residue-property plots

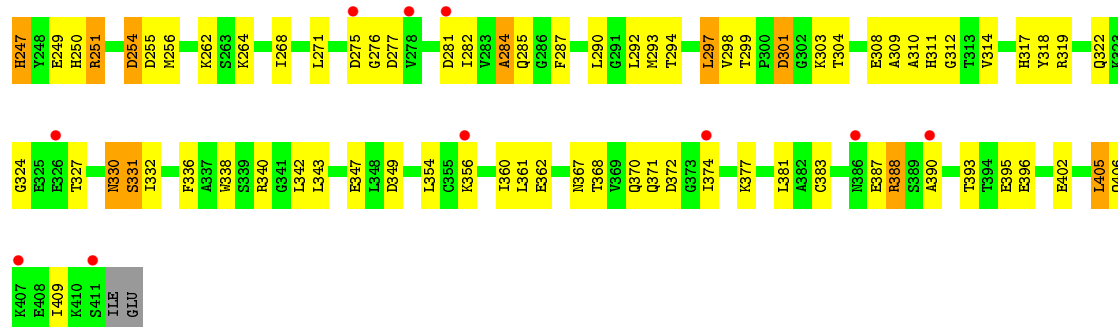
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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]

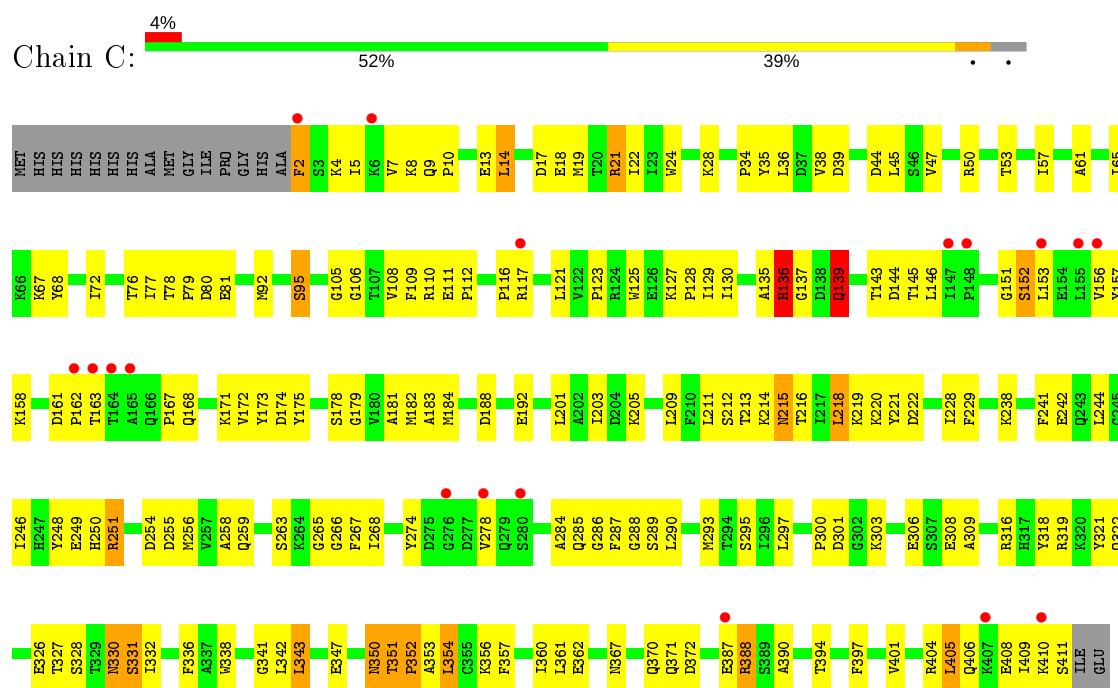


• Molecule 1: Isocitrate dehydrogenase [NADP]

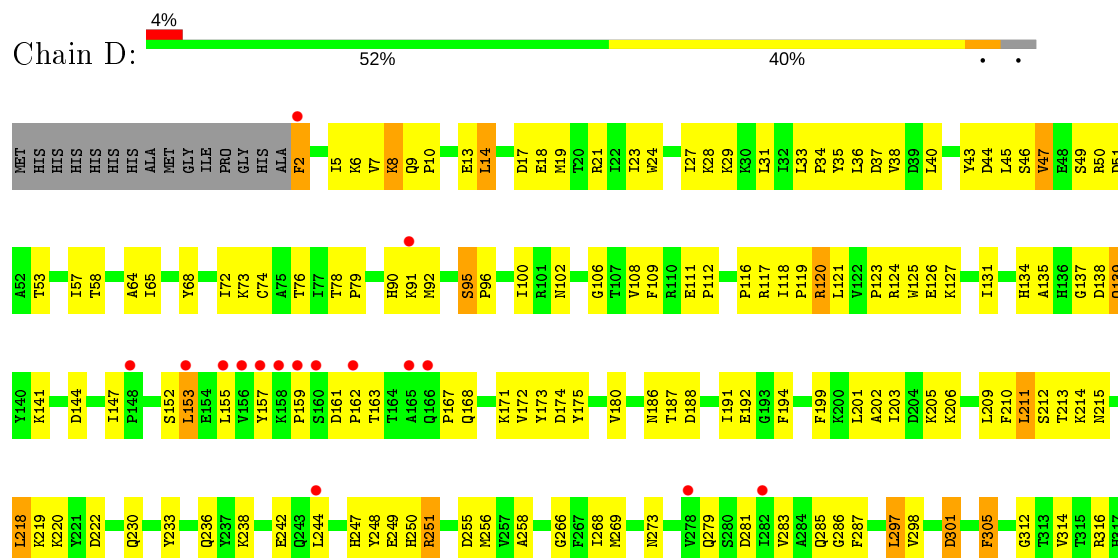


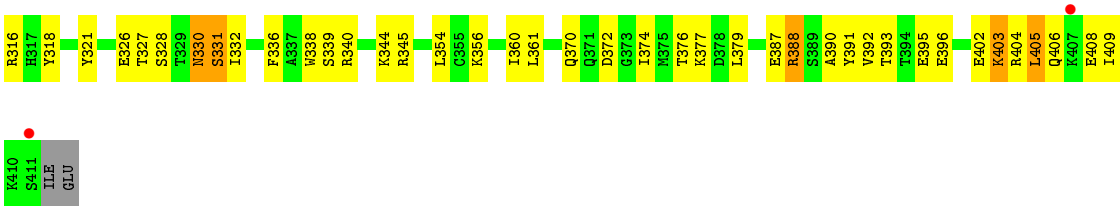


• Molecule 1: Isocitrate dehydrogenase [NADP]



• Molecule 1: Isocitrate dehydrogenase [NADP]





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.42Å 99.63Å 129.95Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	49.73 – 2.70 49.73 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.73-2.70) 98.1 (49.73-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.285 0.216 , 0.218	Depositor DCC
R_{free} test set	3723 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20069	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, CA, 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	0/3311	0.67	1/4466 (0.0%)
1	B	0.37	0/3311	0.66	1/4466 (0.0%)
1	C	0.39	0/3311	0.68	1/4466 (0.0%)
1	D	0.39	0/3311	0.68	0/4466
1	E	0.37	0/3311	0.66	1/4466 (0.0%)
1	F	0.38	0/3311	0.68	1/4466 (0.0%)
All	All	0.38	0/19866	0.67	5/26796 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	HIS	N-CA-C	6.19	127.72	111.00
1	B	136	HIS	N-CA-C	6.15	127.60	111.00
1	F	136	HIS	N-CA-C	5.86	126.81	111.00
1	E	136	HIS	N-CA-C	5.44	125.69	111.00
1	C	136	HIS	N-CA-C	5.27	125.24	111.00

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	3248	0	3291	176	0
1	B	3248	0	3291	188	0
1	C	3248	0	3291	187	0
1	D	3248	0	3291	180	0
1	E	3248	0	3291	178	0
1	F	3248	0	3291	179	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	48	0	26	13	0
3	B	48	0	26	13	0
3	C	48	0	26	12	0
3	D	48	0	26	12	0
3	E	48	0	26	12	0
3	F	48	0	26	11	0
4	A	10	0	4	7	0
4	B	10	0	4	6	0
4	C	10	0	4	6	0
4	D	10	0	4	5	0
4	E	10	0	4	6	0
4	F	10	0	4	5	0
5	A	26	0	0	4	0
5	B	22	0	0	2	0
5	C	47	0	0	1	0
5	D	49	0	0	4	0
5	E	30	0	0	4	0
5	F	53	0	0	9	0
All	All	20069	0	19926	1056	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 27.

All (1056) 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:E:7:VAL:HG21	1:E:38:VAL:HG12	1.39	1.02
1:F:213:THR:HG23	1:F:215:ASN:H	1.27	0.98
1:E:53:THR:HG21	1:E:57:ILE:HG22	1.48	0.96
1:C:301:ASP:HB3	1:C:303:LYS:HG2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HD12	1:E:172:VAL:HB	1.47	0.95
1:E:116:PRO:HB2	1:E:370:GLN:HE22	1.32	0.95
1:F:405:LEU:HD22	1:F:409:ILE:HD11	1.47	0.94
1:C:327:THR:HG22	1:C:394:THR:OG1	1.69	0.93
1:D:7:VAL:HG21	1:D:38:VAL:HG12	1.50	0.93
1:E:327:THR:HG22	1:E:394:THR:OG1	1.69	0.93
1:A:319:ARG:HH11	1:A:322:GLN:HE22	1.17	0.92
1:E:10:PRO:HG2	1:E:68:TYR:CD2	2.04	0.91
1:A:405:LEU:HD22	1:A:409:ILE:HD11	1.52	0.91
3:C:1301:NDP:H42N	4:C:1302:AKG:H41	1.53	0.91
1:C:213:THR:HG23	1:C:222:ASP:HB3	1.54	0.89
1:F:7:VAL:HG21	1:F:38:VAL:HG12	1.52	0.89
1:B:319:ARG:HH11	1:B:322:GLN:NE2	1.71	0.89
1:B:297:LEU:HD12	1:B:298:VAL:N	1.88	0.88
1:C:319:ARG:HH11	1:C:322:GLN:NE2	1.70	0.88
1:D:213:THR:HG23	1:D:222:ASP:HB3	1.55	0.88
1:B:213:THR:HG22	1:B:215:ASN:H	1.36	0.87
1:F:116:PRO:HB2	1:F:370:GLN:HE22	1.38	0.87
1:B:319:ARG:NH1	1:B:322:GLN:HE22	1.71	0.87
1:C:36:LEU:HB3	1:C:38:VAL:HG13	1.58	0.86
1:F:405:LEU:O	1:F:409:ILE:HG13	1.76	0.86
1:B:116:PRO:HB2	1:B:370:GLN:HE22	1.39	0.86
1:C:405:LEU:HD22	1:C:409:ILE:HD11	1.58	0.85
1:E:301:ASP:HB3	1:E:303:LYS:HG2	1.58	0.85
1:B:294:THR:HG21	1:B:340:ARG:HH12	1.42	0.85
1:A:213:THR:HG23	1:A:222:ASP:HB3	1.59	0.85
1:B:330:ASN:ND2	1:B:332:ILE:H	1.74	0.85
1:A:319:ARG:HH11	1:A:322:GLN:NE2	1.75	0.84
1:D:24:TRP:HH2	1:D:72:ILE:HG22	1.42	0.84
1:B:319:ARG:HH11	1:B:322:GLN:HE22	0.86	0.84
1:E:171:LYS:HE2	1:E:174:ASP:OD1	1.76	0.83
1:A:130:ILE:HB	1:A:268:ILE:HG12	1.60	0.83
1:B:405:LEU:HD22	1:B:409:ILE:HD11	1.59	0.83
3:A:1101:NDP:P2B	3:A:1101:NDP:HO3A	2.02	0.82
3:A:1101:NDP:H42N	4:A:1102:AKG:H41	1.61	0.82
1:B:121:LEU:HD12	1:B:285:GLN:O	1.80	0.82
1:E:123:PRO:HG2	1:F:123:PRO:HG2	1.62	0.81
1:C:213:THR:HG22	1:C:215:ASN:H	1.45	0.81
3:F:1601:NDP:H42N	4:F:1602:AKG:H42	1.63	0.81
1:A:405:LEU:O	1:A:409:ILE:HG13	1.80	0.80
3:C:1301:NDP:P2B	3:C:1301:NDP:O3B	2.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:O	1:B:388:ARG:HD3	1.82	0.80
1:E:7:VAL:CG2	1:E:38:VAL:HG12	2.12	0.80
1:B:319:ARG:HD3	1:B:322:GLN:NE2	1.97	0.79
1:C:53:THR:HG21	1:C:57:ILE:HG22	1.64	0.79
1:C:213:THR:CG2	1:C:222:ASP:HB3	2.12	0.79
1:E:254:ASP:HB3	1:F:281:ASP:OD1	1.83	0.79
1:D:213:THR:CG2	1:D:222:ASP:HB3	2.13	0.79
3:D:1401:NDP:H42N	4:D:1402:AKG:H41	1.65	0.78
3:A:1101:NDP:O3B	3:A:1101:NDP:P2B	2.42	0.78
1:E:10:PRO:HG2	1:E:68:TYR:HD2	1.45	0.78
1:B:301:ASP:HB3	1:B:303:LYS:HG2	1.66	0.78
1:B:213:THR:HB	1:B:250:HIS:NE2	1.99	0.78
1:C:116:PRO:HB2	1:C:370:GLN:HE22	1.49	0.78
1:B:213:THR:HG23	1:B:222:ASP:HB3	1.66	0.78
3:F:1601:NDP:C4N	4:F:1602:AKG:H42	2.14	0.77
3:A:1101:NDP:H42N	4:A:1102:AKG:C4	2.14	0.77
3:C:1301:NDP:H42N	4:C:1302:AKG:C4	2.14	0.77
1:D:117:ARG:H	1:D:370:GLN:HE22	1.33	0.77
3:B:1201:NDP:P2B	3:B:1201:NDP:O3B	2.43	0.77
1:C:319:ARG:HH11	1:C:322:GLN:HE22	1.33	0.77
1:B:367:ASN:HB3	1:B:371:GLN:HG3	1.65	0.76
1:D:7:VAL:CG2	1:D:38:VAL:HG12	2.13	0.76
3:C:1301:NDP:P2B	3:C:1301:NDP:HO3A	2.08	0.76
1:C:251:ARG:NE	1:D:316:ARG:HH22	1.83	0.76
1:F:7:VAL:CG2	1:F:38:VAL:HG12	2.15	0.76
1:F:153:LEU:HD12	1:F:172:VAL:HB	1.68	0.75
1:B:387:GLU:HG3	1:B:390:ALA:HB2	1.69	0.75
1:E:4:LYS:HE2	1:E:34:PRO:O	1.85	0.75
1:F:213:THR:HG23	1:F:214:LYS:N	2.02	0.74
1:D:323:LYS:HE3	1:D:325:GLU:OE2	1.87	0.74
1:B:7:VAL:HG21	1:B:38:VAL:HG12	1.70	0.74
3:E:1501:NDP:C4N	4:E:1502:AKG:H42	2.17	0.74
1:A:116:PRO:HB2	1:A:370:GLN:HE22	1.52	0.74
1:E:405:LEU:O	1:E:409:ILE:HG13	1.88	0.74
1:C:35:TYR:CE2	1:C:409:ILE:HD13	2.23	0.74
1:E:356:LYS:O	1:E:360:ILE:HG13	1.88	0.74
1:E:327:THR:HG22	1:E:394:THR:HG1	1.51	0.73
1:E:196:HIS:O	1:E:200:LYS:HG3	1.89	0.73
1:E:202:ALA:HA	1:E:268:ILE:HD12	1.71	0.73
1:B:330:ASN:HD21	1:B:332:ILE:HG13	1.51	0.73
1:B:330:ASN:HD22	1:B:332:ILE:H	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:TRP:HH2	1:C:72:ILE:HG22	1.52	0.73
1:D:297:LEU:HD12	1:D:298:VAL:N	2.04	0.73
1:D:108:VAL:HG23	1:D:135:ALA:HB2	1.69	0.73
1:C:116:PRO:HD2	1:C:370:GLN:NE2	2.03	0.73
1:F:10:PRO:HG2	1:F:68:TYR:CD2	2.23	0.73
1:B:53:THR:HG21	1:B:57:ILE:HG22	1.70	0.72
1:D:330:ASN:HD21	1:D:332:ILE:CG1	2.02	0.72
1:C:24:TRP:CH2	1:C:72:ILE:HG22	2.24	0.72
1:D:238:LYS:O	1:D:242:GLU:HG3	1.89	0.72
1:D:24:TRP:CH2	1:D:72:ILE:HG22	2.25	0.72
1:D:201:LEU:CD2	1:D:205:LYS:HG3	2.19	0.72
1:E:121:LEU:HD13	1:F:262:LYS:HA	1.71	0.72
1:C:330:ASN:HD21	1:C:332:ILE:HG13	1.53	0.72
1:F:53:THR:HG21	1:F:57:ILE:HG22	1.70	0.71
1:E:323:LYS:HE3	1:E:325:GLU:OE2	1.90	0.71
1:C:44:ASP:O	1:C:57:ILE:HD13	1.90	0.71
1:E:146:LEU:CD1	1:F:220:LYS:HB3	2.20	0.71
3:F:1601:NDP:H42N	4:F:1602:AKG:C4	2.19	0.71
1:E:31:LEU:HD22	1:E:405:LEU:HD12	1.73	0.71
1:A:188:ASP:OD1	1:A:228:ILE:HD11	1.91	0.71
1:B:294:THR:HG21	1:B:340:ARG:NH1	2.06	0.71
1:F:224:ARG:NH1	1:F:228:ILE:HG13	2.05	0.71
1:B:213:THR:CG2	1:B:214:LYS:N	2.53	0.70
1:B:79:PRO:HG2	1:B:93:TRP:O	1.91	0.70
1:D:330:ASN:HD21	1:D:332:ILE:HG13	1.55	0.70
1:E:109:PHE:CE1	1:E:201:LEU:HD12	2.26	0.70
1:F:28:LYS:HE3	5:F:1623:HOH:O	1.91	0.70
3:B:1201:NDP:H42N	4:B:1202:AKG:C4	2.21	0.70
1:C:5:ILE:HB	1:C:36:LEU:HD23	1.73	0.70
1:E:213:THR:HG23	1:E:214:LYS:N	2.07	0.70
1:B:116:PRO:HD2	1:B:370:GLN:NE2	2.06	0.70
1:C:254:ASP:HB3	1:D:281:ASP:OD1	1.92	0.70
1:F:102:ASN:HB2	5:F:1654:HOH:O	1.92	0.70
1:F:139:GLN:HA	1:F:142:ALA:HB2	1.74	0.69
1:D:336:PHE:CE2	1:D:362:GLU:HG2	2.27	0.69
3:C:1301:NDP:C4N	4:C:1302:AKG:H41	2.22	0.69
1:C:10:PRO:HG2	1:C:68:TYR:CD2	2.27	0.69
1:B:213:THR:HG22	1:B:215:ASN:N	2.08	0.69
1:D:36:LEU:HB3	1:D:38:VAL:HG13	1.72	0.69
1:B:319:ARG:HA	1:B:322:GLN:HE21	1.56	0.69
1:E:100:ILE:HG21	1:E:306:GLU:OE2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:THR:HG23	1:F:215:ASN:N	2.04	0.69
1:F:117:ARG:HB2	1:F:370:GLN:OE1	1.93	0.69
1:A:53:THR:HG21	1:A:57:ILE:HG22	1.75	0.68
1:B:213:THR:CG2	1:B:222:ASP:HB3	2.23	0.68
1:C:19:MET:CE	1:C:318:TYR:HA	2.23	0.68
1:A:116:PRO:HB2	1:A:370:GLN:NE2	2.08	0.68
1:B:175:TYR:OH	1:B:181:ALA:HB2	1.92	0.68
1:B:116:PRO:HD2	1:B:370:GLN:HE21	1.58	0.68
1:B:201:LEU:O	1:B:201:LEU:HD23	1.94	0.68
1:C:405:LEU:HD22	1:C:409:ILE:CD1	2.24	0.68
1:F:330:ASN:HD21	1:F:332:ILE:HG13	1.57	0.68
1:A:323:LYS:HE3	1:A:325:GLU:OE2	1.93	0.68
1:D:213:THR:HB	1:D:250:HIS:NE2	2.09	0.68
1:B:7:VAL:CG2	1:B:38:VAL:HG12	2.23	0.68
1:A:10:PRO:HG2	1:A:68:TYR:CD2	2.29	0.67
1:C:157:TYR:HB3	1:C:168:GLN:HB2	1.75	0.67
3:E:1501:NDP:H42N	4:E:1502:AKG:H42	1.77	0.67
1:C:213:THR:HB	1:C:250:HIS:NE2	2.10	0.67
1:F:356:LYS:O	1:F:360:ILE:HG13	1.95	0.67
1:B:405:LEU:O	1:B:409:ILE:HG13	1.95	0.67
1:F:213:THR:CG2	1:F:215:ASN:H	2.05	0.67
1:B:116:PRO:HB2	1:B:370:GLN:NE2	2.08	0.67
1:C:301:ASP:CB	1:C:303:LYS:HG2	2.23	0.67
1:E:301:ASP:HB3	1:E:303:LYS:CG	2.25	0.67
1:C:171:LYS:HE2	1:C:174:ASP:OD1	1.94	0.67
1:A:327:THR:HG22	1:A:394:THR:OG1	1.94	0.67
1:E:188:ASP:O	1:E:192:GLU:HG3	1.95	0.67
1:A:125:TRP:HZ3	1:A:286:GLY:HA3	1.60	0.66
1:B:330:ASN:HD21	1:B:332:ILE:CG1	2.08	0.66
1:C:218:LEU:HD11	1:D:139:GLN:HB2	1.77	0.66
1:A:248:TYR:O	1:A:249:GLU:HB2	1.95	0.66
1:A:241:PHE:CD2	1:A:246:ILE:HG13	2.31	0.66
1:C:188:ASP:OD1	1:C:228:ILE:HD11	1.95	0.66
1:A:213:THR:CG2	1:A:222:ASP:HB3	2.24	0.66
3:F:1601:NDP:O3B	3:F:1601:NDP:P2B	2.53	0.66
1:B:238:LYS:O	1:B:242:GLU:HG3	1.96	0.66
1:D:19:MET:HE1	1:D:318:TYR:HA	1.77	0.66
1:E:388:ARG:HD3	1:E:388:ARG:O	1.96	0.66
1:C:297:LEU:HB3	1:C:306:GLU:HB3	1.78	0.66
1:E:127:LYS:HD3	1:E:266:GLY:HA3	1.78	0.66
1:E:92:MET:HG2	1:F:219:LYS:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:THR:HG21	1:E:57:ILE:CG2	2.24	0.65
1:F:405:LEU:CD2	1:F:409:ILE:HD11	2.22	0.65
1:D:327:THR:HG22	1:D:394:THR:OG1	1.96	0.65
1:D:201:LEU:HD23	1:D:205:LYS:HG3	1.78	0.65
1:D:111:GLU:HB2	1:D:112:PRO:HD2	1.76	0.65
1:B:247:HIS:HB3	5:B:1211:HOH:O	1.97	0.65
1:C:145:THR:HA	1:D:220:LYS:HD3	1.79	0.65
1:E:301:ASP:CB	1:E:303:LYS:HG2	2.24	0.65
1:F:49:SER:O	1:F:53:THR:HG22	1.97	0.65
1:C:14:LEU:HD23	1:C:14:LEU:N	2.11	0.65
1:C:7:VAL:CG2	1:C:38:VAL:HG12	2.27	0.65
1:F:138:ASP:HB3	1:F:139:GLN:OE1	1.97	0.65
1:C:72:ILE:HD11	1:C:341:GLY:HA3	1.79	0.65
1:A:109:PHE:CE1	1:A:201:LEU:HD12	2.32	0.64
1:A:19:MET:HE1	1:A:318:TYR:HA	1.79	0.64
3:B:1201:NDP:H42N	4:B:1202:AKG:H41	1.78	0.64
1:B:67:LYS:HD3	1:B:68:TYR:CE1	2.33	0.64
4:F:1602:AKG:H32	5:F:1618:HOH:O	1.97	0.64
3:F:1601:NDP:P2B	3:F:1601:NDP:HO3A	2.21	0.64
1:F:330:ASN:HD21	1:F:332:ILE:CG1	2.10	0.64
1:A:102:ASN:ND2	1:A:141:LYS:HG3	2.12	0.64
1:B:319:ARG:HD3	1:B:322:GLN:HE21	1.60	0.64
1:C:319:ARG:HD3	1:C:322:GLN:HE21	1.62	0.64
1:F:308:GLU:HG3	1:F:309:ALA:O	1.98	0.64
1:A:7:VAL:HG21	1:A:38:VAL:HG12	1.80	0.64
1:B:53:THR:HG21	1:B:57:ILE:CG2	2.27	0.64
1:D:76:THR:O	3:D:1401:NDP:H2N	1.98	0.64
1:E:116:PRO:CB	1:E:370:GLN:HE22	2.09	0.64
1:F:393:THR:HG23	5:F:1639:HOH:O	1.96	0.64
1:C:251:ARG:NE	1:D:316:ARG:NH2	2.46	0.63
1:A:343:LEU:HG	1:A:358:ALA:CB	2.27	0.63
1:C:78:THR:OG1	1:C:95:SER:HB2	1.98	0.63
1:A:254:ASP:HB3	1:B:281:ASP:OD1	1.98	0.63
1:B:10:PRO:HG2	1:B:68:TYR:CD2	2.34	0.63
1:D:213:THR:HG22	1:D:215:ASN:H	1.62	0.63
1:D:117:ARG:N	1:D:370:GLN:HE22	1.96	0.63
1:A:116:PRO:HD2	1:A:370:GLN:NE2	2.13	0.63
1:D:49:SER:O	1:D:53:THR:HG22	1.97	0.63
3:E:1501:NDP:P2B	3:E:1501:NDP:HO3A	2.21	0.63
1:F:251:ARG:HD2	1:F:255:ASP:OD1	1.99	0.63
3:A:1101:NDP:C4N	4:A:1102:AKG:H41	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:CG2	1:A:214:LYS:N	2.61	0.63
1:A:31:LEU:HD22	1:A:405:LEU:HD12	1.80	0.63
1:D:172:VAL:O	1:D:173:TYR:HB2	1.99	0.63
1:D:6:LYS:HA	1:D:37:ASP:HB3	1.81	0.63
1:A:68:TYR:O	1:A:345:ARG:NH1	2.30	0.62
1:C:92:MET:CE	1:D:219:LYS:HD3	2.29	0.62
1:B:7:VAL:HG21	1:B:38:VAL:CG1	2.29	0.62
1:C:108:VAL:HG23	1:C:135:ALA:HB2	1.81	0.62
3:C:1301:NDP:H42N	4:C:1302:AKG:C2	2.29	0.62
1:D:206:LYS:HG2	1:D:244:LEU:HD22	1.81	0.62
1:B:20:THR:OG1	1:B:75:ALA:HB3	2.00	0.62
1:A:153:LEU:HD12	1:A:172:VAL:HB	1.82	0.62
1:B:35:TYR:CE2	1:B:409:ILE:HD13	2.33	0.62
1:A:228:ILE:O	1:A:232:VAL:HG23	1.99	0.62
1:B:330:ASN:HD22	1:B:331:SER:N	1.98	0.62
1:C:388:ARG:O	1:C:388:ARG:HD3	2.00	0.62
1:D:213:THR:HG22	1:D:215:ASN:N	2.15	0.62
1:C:7:VAL:HG21	1:C:38:VAL:HG12	1.82	0.61
1:D:387:GLU:HG3	1:D:390:ALA:HB2	1.82	0.61
1:B:251:ARG:HG3	1:B:251:ARG:HH11	1.65	0.61
1:B:116:PRO:CB	1:B:370:GLN:HE22	2.12	0.61
1:E:372:ASP:OD2	1:E:404:ARG:NE	2.32	0.61
1:B:340:ARG:HH11	1:B:340:ARG:HG3	1.65	0.61
1:C:356:LYS:O	1:C:360:ILE:HG13	1.99	0.61
3:D:1401:NDP:O3B	3:D:1401:NDP:P2B	2.57	0.61
1:E:372:ASP:HB2	1:E:374:ILE:HD12	1.82	0.61
1:F:78:THR:OG1	1:F:95:SER:HB2	2.00	0.61
1:B:21:ARG:NH2	1:B:44:ASP:OD1	2.34	0.61
1:E:38:VAL:HG23	1:E:40:LEU:HG	1.83	0.61
1:F:81:GLU:HB2	5:F:1650:HOH:O	1.99	0.61
1:E:213:THR:CG2	1:E:215:ASN:H	2.14	0.61
1:F:327:THR:HG22	1:F:328:SER:N	2.14	0.61
3:D:1401:NDP:C4N	4:D:1402:AKG:H41	2.30	0.61
1:F:336:PHE:HA	1:F:339:SER:OG	2.01	0.61
1:B:13:GLU:C	1:B:14:LEU:HD23	2.20	0.61
1:D:29:LYS:O	1:D:34:PRO:HD3	2.00	0.61
3:E:1501:NDP:H42N	4:E:1502:AKG:C4	2.30	0.61
1:C:145:THR:HA	1:D:220:LYS:CD	2.31	0.61
1:E:387:GLU:HG3	1:E:390:ALA:HB2	1.82	0.61
1:F:175:TYR:OH	1:F:181:ALA:HB2	2.00	0.61
1:A:248:TYR:CG	1:A:249:GLU:N	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:HE1	1:A:274:TYR:HA	1.65	0.60
1:E:349:ASP:O	1:E:350:ASN:HB2	2.00	0.60
3:B:1201:NDP:H42N	4:B:1202:AKG:C2	2.31	0.60
1:A:220:LYS:HB3	1:B:146:LEU:HD12	1.83	0.60
1:C:220:LYS:HD2	1:D:144:ASP:O	2.01	0.60
1:C:343:LEU:O	1:C:347:GLU:HG3	2.01	0.60
1:D:203:ILE:HG23	1:D:244:LEU:HD11	1.81	0.60
1:F:10:PRO:HG2	1:F:68:TYR:HD2	1.66	0.60
1:A:187:THR:O	1:A:191:ILE:HG13	2.00	0.60
1:A:299:THR:OG1	1:A:304:THR:HB	2.01	0.60
3:C:1301:NDP:O1X	3:C:1301:NDP:O3B	2.18	0.60
1:E:8:LYS:HB3	1:E:349:ASP:HB3	1.81	0.60
1:A:50:ARG:HA	1:A:53:THR:HG22	1.81	0.60
1:C:213:THR:HG22	1:C:215:ASN:N	2.16	0.60
1:C:53:THR:HG21	1:C:57:ILE:CG2	2.31	0.60
1:D:343:LEU:O	1:D:347:GLU:HG3	2.01	0.60
1:E:171:LYS:HE2	1:E:174:ASP:CG	2.20	0.60
1:A:2:PHE:CD2	1:A:2:PHE:N	2.67	0.60
1:B:377:LYS:HE2	1:B:381:LEU:HD11	1.83	0.60
1:D:124:ARG:HB3	5:D:1421:HOH:O	2.01	0.60
1:E:301:ASP:OD2	1:E:303:LYS:HD3	2.02	0.60
1:C:19:MET:HE2	1:C:318:TYR:HA	1.82	0.60
1:C:285:GLN:HG2	1:D:258:ALA:O	2.02	0.60
1:A:155:LEU:HD23	1:B:183:ALA:HB2	1.83	0.60
1:E:301:ASP:HB3	1:E:303:LYS:CD	2.32	0.60
1:D:116:PRO:HB2	1:D:370:GLN:NE2	2.17	0.60
1:A:301:ASP:CB	1:A:303:LYS:HG2	2.32	0.59
1:B:405:LEU:HD22	1:B:409:ILE:CD1	2.32	0.59
1:E:35:TYR:CE2	1:E:409:ILE:HD12	2.37	0.59
1:E:81:GLU:HB2	5:E:1527:HOH:O	2.02	0.59
1:D:78:THR:OG1	1:D:95:SER:HB2	2.02	0.59
3:E:1501:NDP:P2B	3:E:1501:NDP:O3B	2.60	0.59
1:A:319:ARG:NH1	1:A:322:GLN:HE22	1.93	0.59
1:C:144:ASP:OD2	1:D:220:LYS:HB2	2.02	0.59
1:F:121:LEU:HD12	1:F:285:GLN:O	2.03	0.59
1:F:201:LEU:HD22	1:F:268:ILE:HD11	1.83	0.59
1:B:251:ARG:NH1	1:B:251:ARG:HG3	2.17	0.59
1:E:338:TRP:O	1:E:342:LEU:HG	2.01	0.59
1:A:213:THR:HG22	1:A:215:ASN:H	1.66	0.59
1:B:356:LYS:O	1:B:360:ILE:HG13	2.03	0.59
1:D:330:ASN:ND2	1:D:332:ILE:HG13	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:ALA:HA	1:F:229:PHE:CZ	2.37	0.59
1:A:146:LEU:CD1	1:B:220:LYS:HB3	2.33	0.59
1:B:297:LEU:C	1:B:297:LEU:HD12	2.22	0.59
1:E:131:ILE:HD13	1:E:269:MET:HB2	1.83	0.59
1:B:402:GLU:O	1:B:406:GLN:HG3	2.02	0.59
1:C:116:PRO:CB	1:C:370:GLN:HE22	2.16	0.59
1:C:251:ARG:CD	1:D:316:ARG:HH22	2.15	0.59
1:E:409:ILE:C	1:E:411:SER:H	2.04	0.59
1:C:182:MET:HE1	1:D:218:LEU:HD21	1.83	0.59
1:D:330:ASN:ND2	1:D:332:ILE:H	2.01	0.59
1:D:35:TYR:CE2	1:D:409:ILE:HD12	2.38	0.59
1:E:405:LEU:HD22	1:E:409:ILE:HD11	1.85	0.59
1:B:44:ASP:O	1:B:57:ILE:HD13	2.03	0.58
1:E:251:ARG:HD3	1:F:316:ARG:HH22	1.68	0.58
1:E:352:PRO:O	1:E:356:LYS:HG3	2.03	0.58
3:E:1501:NDP:H42N	4:E:1502:AKG:C2	2.33	0.58
1:D:153:LEU:HD12	1:D:172:VAL:HB	1.85	0.58
1:D:211:LEU:HD22	1:D:212:SER:N	2.18	0.58
1:D:336:PHE:CZ	1:D:362:GLU:HG2	2.38	0.58
3:F:1601:NDP:O3X	3:F:1601:NDP:H3B	2.04	0.58
1:C:2:PHE:CD2	1:C:2:PHE:N	2.70	0.58
1:E:219:LYS:HD3	1:F:92:MET:HE3	1.84	0.58
1:E:330:ASN:HD21	1:E:332:ILE:HG13	1.68	0.58
1:F:301:ASP:HB3	1:F:303:LYS:CD	2.32	0.58
1:B:330:ASN:HD22	1:B:330:ASN:C	2.07	0.58
1:C:330:ASN:HD22	1:C:331:SER:N	2.02	0.58
1:E:213:THR:CG2	1:E:214:LYS:N	2.66	0.58
1:C:144:ASP:O	1:D:220:LYS:HD2	2.04	0.58
1:F:147:ILE:HG13	1:F:175:TYR:CZ	2.38	0.58
1:B:213:THR:HG22	1:B:214:LYS:N	2.17	0.58
1:E:319:ARG:HH11	1:E:322:GLN:NE2	2.02	0.58
1:F:405:LEU:HD22	1:F:409:ILE:CD1	2.27	0.58
1:C:213:THR:HG21	1:C:215:ASN:HB3	1.86	0.58
1:C:182:MET:HE1	1:D:218:LEU:CD2	2.34	0.58
1:D:116:PRO:HD2	1:D:370:GLN:HE21	1.67	0.58
3:E:1501:NDP:C5N	4:E:1502:AKG:H42	2.34	0.58
1:A:13:GLU:C	1:A:14:LEU:HD23	2.24	0.58
1:B:213:THR:HG23	1:B:214:LYS:H	1.68	0.58
1:C:251:ARG:HE	1:D:316:ARG:NH2	2.02	0.58
1:F:153:LEU:HD12	1:F:172:VAL:CB	2.34	0.58
1:A:19:MET:CE	1:A:318:TYR:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LEU:HD23	1:D:201:LEU:O	2.03	0.57
1:D:213:THR:CG2	1:D:214:LYS:N	2.67	0.57
1:C:213:THR:CG2	1:C:215:ASN:HB3	2.35	0.57
1:C:203:ILE:HG23	1:C:244:LEU:HD11	1.86	0.57
1:C:50:ARG:HA	1:C:53:THR:HG22	1.86	0.57
1:D:14:LEU:HD21	1:D:65:ILE:HD11	1.85	0.57
1:A:116:PRO:HD2	1:A:370:GLN:HE21	1.68	0.57
1:B:108:VAL:HG23	1:B:135:ALA:HB2	1.87	0.57
1:D:53:THR:HG21	1:D:57:ILE:HB	1.86	0.57
1:E:119:PRO:C	1:E:120:ARG:HG3	2.24	0.57
1:B:117:ARG:HB2	1:B:370:GLN:OE1	2.03	0.57
1:B:16:GLY:HA3	1:B:75:ALA:O	2.05	0.57
1:F:312:GLY:N	3:F:1601:NDP:O1A	2.35	0.57
1:B:301:ASP:CB	1:B:303:LYS:HG2	2.34	0.57
1:D:201:LEU:HD21	1:D:205:LYS:HG3	1.86	0.57
1:A:404:ARG:NH1	1:A:408:GLU:OE2	2.33	0.57
1:C:213:THR:CG2	1:C:214:LYS:N	2.67	0.57
1:F:330:ASN:HD22	1:F:332:ILE:H	1.52	0.57
1:B:166:GLN:HB3	1:B:167:PRO:HD2	1.86	0.56
1:C:178:SER:O	1:D:188:ASP:HB2	2.04	0.56
1:E:281:ASP:OD1	1:F:254:ASP:HB3	2.05	0.56
1:E:219:LYS:HB3	1:F:92:MET:HE3	1.85	0.56
1:A:92:MET:CE	1:B:219:LYS:HB3	2.36	0.56
1:E:87:PHE:HB2	1:E:89:LEU:HD21	1.86	0.56
1:C:201:LEU:HD22	1:C:268:ILE:HD11	1.88	0.56
1:C:404:ARG:HB2	5:C:1330:HOH:O	2.05	0.56
1:E:251:ARG:HD3	1:F:316:ARG:NH2	2.20	0.56
1:E:124:ARG:HH11	1:F:121:LEU:HD21	1.71	0.56
1:C:319:ARG:NH1	1:C:322:GLN:HE22	2.04	0.56
1:E:24:TRP:CH2	1:E:72:ILE:HG22	2.41	0.56
1:F:172:VAL:O	1:F:173:TYR:HB2	2.05	0.56
1:B:271:LEU:HB3	1:B:275:ASP:HB2	1.86	0.56
1:E:212:SER:OG	1:E:256:MET:HG2	2.05	0.56
1:A:76:THR:O	3:A:1101:NDP:H2N	2.06	0.56
1:A:160:SER:O	1:A:162:PRO:HD3	2.06	0.56
1:D:19:MET:HE3	1:D:327:THR:HG21	1.88	0.56
1:E:164:THR:HG22	1:E:164:THR:O	2.06	0.56
1:B:308:GLU:HG3	1:B:309:ALA:O	2.05	0.56
1:D:120:ARG:CZ	1:D:125:TRP:O	2.54	0.56
1:F:330:ASN:ND2	1:F:332:ILE:H	2.04	0.56
1:B:138:ASP:HB3	1:B:139:GLN:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:C	1:E:154:GLU:HG3	2.26	0.56
1:C:330:ASN:HD21	1:C:332:ILE:CG1	2.17	0.56
3:D:1401:NDP:H42N	4:D:1402:AKG:C4	2.33	0.55
1:D:2:PHE:CD2	1:D:2:PHE:N	2.74	0.55
1:F:224:ARG:NH1	1:F:228:ILE:CG1	2.69	0.55
1:B:161:ASP:O	1:B:163:THR:N	2.38	0.55
1:D:117:ARG:H	1:D:370:GLN:NE2	2.03	0.55
1:F:99:THR:O	1:F:103:ILE:HG13	2.05	0.55
3:F:1601:NDP:O3X	3:F:1601:NDP:C3B	2.53	0.55
1:F:230:GLN:HE21	1:F:234:GLU:CG	2.20	0.55
3:A:1101:NDP:C4N	4:A:1102:AKG:C4	2.83	0.55
1:A:147:ILE:HG13	1:A:175:TYR:CZ	2.42	0.55
1:F:301:ASP:HB3	1:F:303:LYS:HG2	1.88	0.55
1:A:10:PRO:HG2	1:A:68:TYR:HD2	1.71	0.55
1:A:308:GLU:HG3	1:A:309:ALA:O	2.06	0.55
3:F:1601:NDP:C5N	4:F:1602:AKG:H42	2.35	0.55
1:F:330:ASN:ND2	1:F:332:ILE:HG13	2.21	0.55
1:A:129:ILE:HG13	1:A:287:PHE:HZ	1.72	0.55
1:D:312:GLY:N	3:D:1401:NDP:O1A	2.37	0.55
1:C:258:ALA:O	1:D:285:GLN:HG2	2.07	0.55
1:E:139:GLN:HA	1:E:142:ALA:HB2	1.87	0.55
1:E:36:LEU:HB3	1:E:38:VAL:HG13	1.88	0.55
1:D:314:VAL:HG12	1:D:314:VAL:O	2.07	0.55
1:A:201:LEU:CD2	1:A:205:LYS:HG3	2.37	0.55
1:B:312:GLY:N	3:B:1201:NDP:O1A	2.36	0.55
1:C:201:LEU:HD23	1:C:201:LEU:O	2.06	0.55
3:D:1401:NDP:O3X	3:D:1401:NDP:H3B	2.07	0.55
1:C:219:LYS:HD3	1:D:92:MET:HE3	1.88	0.55
1:E:279:GLN:O	1:E:283:VAL:HG23	2.06	0.55
1:F:13:GLU:C	1:F:14:LEU:HD23	2.26	0.55
1:C:406:GLN:HA	1:C:409:ILE:HD12	1.88	0.55
1:D:388:ARG:HD3	1:D:388:ARG:O	2.07	0.55
1:D:374:ILE:HG23	1:D:392:VAL:HG11	1.87	0.55
1:F:122:VAL:HG11	1:F:125:TRP:CE2	2.42	0.55
1:A:213:THR:HG23	1:A:214:LYS:H	1.72	0.54
1:A:296:ILE:HD11	1:A:344:LYS:HG3	1.89	0.54
1:B:19:MET:HE3	1:B:327:THR:HG21	1.89	0.54
1:E:144:ASP:OD2	1:F:220:LYS:HB2	2.06	0.54
1:F:36:LEU:HB3	1:F:38:VAL:HG13	1.89	0.54
3:A:1101:NDP:H42N	4:A:1102:AKG:C2	2.37	0.54
3:A:1101:NDP:C5N	4:A:1102:AKG:H42	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HB3	1:A:38:VAL:HG13	1.89	0.54
1:B:105:GLY:O	1:B:297:LEU:HD11	2.07	0.54
1:B:17:ASP:OD1	1:B:46:SER:HA	2.08	0.54
1:B:86:GLU:HG2	1:B:87:PHE:CE1	2.43	0.54
1:C:109:PHE:CE1	1:C:201:LEU:HD12	2.42	0.54
1:C:121:LEU:HD12	1:C:285:GLN:O	2.06	0.54
1:E:367:ASN:HB3	1:E:371:GLN:HG3	1.89	0.54
3:A:1101:NDP:O3X	3:A:1101:NDP:C3B	2.55	0.54
1:A:319:ARG:HD3	1:A:322:GLN:NE2	2.22	0.54
1:E:105:GLY:O	1:E:297:LEU:HD11	2.07	0.54
3:C:1301:NDP:O3X	3:C:1301:NDP:C3B	2.56	0.54
1:C:106:GLY:CA	1:C:300:PRO:HD3	2.37	0.54
1:E:146:LEU:HD12	1:F:220:LYS:HB3	1.90	0.54
1:D:102:ASN:OD1	1:D:141:LYS:HE3	2.08	0.54
1:E:213:THR:HG21	1:E:215:ASN:HB3	1.89	0.54
1:E:372:ASP:CG	1:E:404:ARG:HE	2.11	0.54
1:B:188:ASP:O	1:B:192:GLU:HG3	2.07	0.54
1:E:228:ILE:O	1:E:232:VAL:HG23	2.07	0.54
1:E:24:TRP:HH2	1:E:72:ILE:HG22	1.70	0.54
1:E:330:ASN:HD22	1:E:331:SER:N	2.05	0.54
1:D:117:ARG:CZ	1:D:370:GLN:O	2.56	0.54
1:E:213:THR:HG23	1:E:215:ASN:N	2.22	0.54
1:B:124:ARG:O	1:B:264:LYS:HA	2.07	0.54
1:C:387:GLU:HG3	1:C:390:ALA:HB2	1.90	0.54
1:C:221:TYR:CE1	1:D:180:VAL:HG23	2.43	0.54
1:F:76:THR:O	3:F:1601:NDP:H2N	2.08	0.54
1:A:14:LEU:N	1:A:14:LEU:HD23	2.22	0.53
1:C:116:PRO:HB2	1:C:370:GLN:NE2	2.19	0.53
1:C:201:LEU:HD22	1:C:268:ILE:CD1	2.38	0.53
1:F:117:ARG:CZ	1:F:370:GLN:O	2.56	0.53
1:B:102:ASN:ND2	1:B:141:LYS:HG3	2.23	0.53
1:C:301:ASP:HB3	1:C:303:LYS:CG	2.27	0.53
1:C:36:LEU:HB3	1:C:38:VAL:CG1	2.33	0.53
1:B:213:THR:CG2	1:B:214:LYS:H	2.21	0.53
1:B:7:VAL:CB	1:B:38:VAL:HG12	2.39	0.53
1:B:86:GLU:HG2	1:B:87:PHE:CD1	2.43	0.53
1:C:92:MET:HE3	1:D:219:LYS:HD3	1.90	0.53
3:D:1401:NDP:O3X	3:D:1401:NDP:C3B	2.56	0.53
1:F:50:ARG:HA	1:F:53:THR:HG22	1.90	0.53
1:F:54:SER:HA	1:F:93:TRP:CH2	2.43	0.53
1:A:284:ALA:HB2	1:A:293:MET:SD	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:HD3	1:B:349:ASP:HB3	1.91	0.53
1:C:327:THR:CG2	1:C:394:THR:OG1	2.50	0.53
1:D:199:PHE:CZ	1:D:233:TYR:HB2	2.43	0.53
1:D:27:ILE:HG23	1:D:31:LEU:HD12	1.90	0.53
1:E:73:LYS:HZ3	1:E:76:THR:HG23	1.73	0.53
1:A:220:LYS:HB3	1:B:146:LEU:CD1	2.37	0.53
1:F:238:LYS:O	1:F:242:GLU:HG3	2.09	0.53
1:B:121:LEU:O	1:B:123:PRO:HD3	2.08	0.53
1:B:2:PHE:N	1:B:2:PHE:CD2	2.75	0.53
1:C:259:GLN:NE2	3:D:1401:NDP:O3B	2.41	0.53
1:D:330:ASN:HD22	1:D:331:SER:N	2.06	0.53
1:A:297:LEU:HD12	1:A:298:VAL:N	2.23	0.53
1:B:161:ASP:C	1:B:163:THR:H	2.11	0.53
1:D:279:GLN:O	1:D:283:VAL:HG23	2.08	0.53
1:D:374:ILE:CG2	1:D:392:VAL:HG11	2.39	0.53
3:E:1501:NDP:O3X	3:E:1501:NDP:H3B	2.09	0.53
1:F:213:THR:CG2	1:F:214:LYS:N	2.72	0.53
1:B:56:LYS:O	1:B:59:GLN:HB2	2.08	0.53
1:A:124:ARG:HD3	1:A:262:LYS:O	2.09	0.53
1:B:409:ILE:O	1:B:409:ILE:HG22	2.09	0.53
1:C:127:LYS:HG3	1:C:128:PRO:HD2	1.90	0.53
1:C:21:ARG:NH2	1:C:44:ASP:OD1	2.42	0.53
1:D:330:ASN:HD21	1:D:332:ILE:CD1	2.21	0.53
1:E:319:ARG:HH11	1:E:322:GLN:HE22	1.55	0.53
1:A:109:PHE:CD1	1:A:201:LEU:HD12	2.45	0.52
1:D:330:ASN:HD22	1:D:332:ILE:H	1.56	0.52
1:C:219:LYS:HD3	1:D:92:MET:CE	2.40	0.52
1:D:364:ALA:HA	1:D:408:GLU:OE2	2.10	0.52
1:E:238:LYS:O	1:E:242:GLU:HG3	2.09	0.52
1:C:106:GLY:HA2	1:C:300:PRO:HD3	1.90	0.52
1:C:388:ARG:C	1:C:388:ARG:HD3	2.28	0.52
1:A:301:ASP:HB2	1:A:303:LYS:HG2	1.92	0.52
1:D:305:PHE:N	1:D:305:PHE:CD2	2.78	0.52
1:E:251:ARG:CD	1:F:316:ARG:HH22	2.23	0.52
1:F:12:VAL:HG12	1:F:14:LEU:HD21	1.92	0.52
1:A:24:TRP:CH2	1:A:72:ILE:HG22	2.45	0.52
1:F:393:THR:H	1:F:396:GLU:HB2	1.74	0.52
1:A:213:THR:HG23	1:A:214:LYS:N	2.23	0.52
1:E:213:THR:HG23	1:E:214:LYS:H	1.73	0.52
1:E:316:ARG:HH22	1:F:251:ARG:NE	2.07	0.52
1:F:284:ALA:HB2	1:F:293:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASP:O	1:B:83:ARG:N	2.43	0.52
1:C:213:THR:HG23	1:C:222:ASP:CB	2.34	0.52
1:B:388:ARG:C	1:B:388:ARG:HD3	2.31	0.52
1:C:330:ASN:ND2	1:C:332:ILE:H	2.08	0.52
1:C:117:ARG:HB2	1:C:370:GLN:OE1	2.10	0.52
1:D:117:ARG:HB2	1:D:370:GLN:OE1	2.10	0.52
1:D:397:PHE:O	1:D:401:VAL:HG23	2.10	0.52
1:E:153:LEU:O	1:E:154:GLU:HG3	2.10	0.52
1:A:368:THR:HG22	1:A:374:ILE:HB	1.92	0.51
1:C:284:ALA:HB2	1:C:293:MET:SD	2.49	0.51
1:C:330:ASN:ND2	1:C:332:ILE:HG13	2.22	0.51
1:E:220:LYS:HB3	1:F:146:LEU:HD11	1.90	0.51
1:A:50:ARG:HA	1:A:53:THR:CG2	2.40	0.51
1:A:24:TRP:HH2	1:A:72:ILE:HG22	1.74	0.51
1:C:92:MET:HE2	1:D:219:LYS:HD3	1.91	0.51
1:F:53:THR:HG21	1:F:57:ILE:CG2	2.39	0.51
1:C:183:ALA:HB2	1:D:155:LEU:HD23	1.92	0.51
1:F:201:LEU:HD22	1:F:268:ILE:CD1	2.40	0.51
1:C:251:ARG:CD	1:D:316:ARG:NH2	2.73	0.51
3:E:1501:NDP:O3X	3:E:1501:NDP:C3B	2.58	0.51
1:E:73:LYS:NZ	1:E:76:THR:HG23	2.26	0.51
1:A:7:VAL:CG2	1:A:38:VAL:HG12	2.40	0.51
1:B:116:PRO:CD	1:B:370:GLN:NE2	2.74	0.51
1:B:405:LEU:CD2	1:B:409:ILE:HD11	2.35	0.51
1:C:116:PRO:CD	1:C:370:GLN:NE2	2.74	0.51
1:E:213:THR:HG23	1:E:215:ASN:H	1.76	0.51
1:F:116:PRO:HB2	1:F:370:GLN:NE2	2.18	0.51
1:A:12:VAL:HG12	1:A:14:LEU:HD21	1.93	0.51
1:A:235:ALA:O	1:A:236:GLN:HB3	2.11	0.51
1:E:131:ILE:HG23	1:E:271:LEU:HD12	1.93	0.51
1:E:161:ASP:C	1:E:163:THR:H	2.14	0.51
1:F:146:LEU:N	1:F:146:LEU:HD12	2.26	0.51
1:B:54:SER:HA	1:B:93:TRP:CH2	2.45	0.51
1:C:139:GLN:HB3	1:C:184:MET:CE	2.41	0.51
1:D:297:LEU:HD12	1:D:297:LEU:C	2.29	0.51
1:D:326:GLU:OE1	1:D:388:ARG:NH2	2.37	0.51
1:B:336:PHE:CE2	1:B:362:GLU:HG2	2.46	0.51
1:A:292:LEU:HD11	1:A:379:LEU:HD21	1.91	0.51
1:C:13:GLU:C	1:C:14:LEU:HD23	2.30	0.51
1:C:172:VAL:O	1:C:173:TYR:HB2	2.11	0.51
1:C:326:GLU:CD	1:C:388:ARG:HH21	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:PHE:HD2	1:D:2:PHE:N	2.08	0.51
1:D:405:LEU:O	1:D:409:ILE:HG13	2.11	0.51
1:F:2:PHE:N	1:F:2:PHE:CD2	2.79	0.51
1:E:220:LYS:HB3	1:F:146:LEU:CD1	2.41	0.50
1:F:22:ILE:HD11	1:F:321:TYR:CE2	2.46	0.50
1:A:281:ASP:OD1	1:B:254:ASP:HB3	2.10	0.50
1:E:104:LEU:O	1:E:299:THR:HG22	2.12	0.50
1:E:153:LEU:HB2	1:E:175:TYR:HE1	1.76	0.50
1:A:220:LYS:HD2	1:B:145:THR:HA	1.92	0.50
1:A:370:GLN:HA	1:A:370:GLN:OE1	2.10	0.50
1:C:10:PRO:HB3	1:C:39:ASP:OD2	2.11	0.50
1:D:202:ALA:HA	1:D:268:ILE:HD12	1.94	0.50
1:F:56:LYS:O	1:F:59:GLN:HB2	2.10	0.50
1:D:90:HIS:CD2	1:D:91:LYS:HG3	2.47	0.50
1:B:330:ASN:ND2	1:B:332:ILE:HG13	2.24	0.50
1:E:153:LEU:HD12	1:E:172:VAL:CB	2.31	0.50
1:F:7:VAL:HG21	1:F:38:VAL:CG1	2.34	0.50
1:A:116:PRO:CB	1:A:370:GLN:HE22	2.23	0.50
1:C:201:LEU:HD23	1:C:205:LYS:HG3	1.93	0.50
1:C:241:PHE:CD2	1:C:246:ILE:HG13	2.46	0.50
1:C:9:GLN:OE1	1:C:9:GLN:HA	2.12	0.50
1:D:403:LYS:O	1:D:407:LYS:HG2	2.11	0.50
1:E:182:MET:HE1	1:F:218:LEU:HD21	1.94	0.50
1:B:201:LEU:HD22	1:B:268:ILE:CD1	2.42	0.50
1:D:120:ARG:NH1	5:D:1422:HOH:O	2.44	0.50
1:F:127:LYS:HG3	1:F:128:PRO:HD2	1.93	0.50
1:A:153:LEU:HD21	1:B:155:LEU:HD11	1.93	0.50
1:B:330:ASN:HD21	1:B:332:ILE:CB	2.24	0.50
1:B:76:THR:O	3:B:1201:NDP:H2N	2.12	0.50
1:C:111:GLU:HB2	1:C:112:PRO:HD2	1.94	0.50
1:D:301:ASP:N	1:D:301:ASP:OD1	2.42	0.50
1:D:73:LYS:HG2	1:D:74:CYS:O	2.12	0.50
1:F:26:LYS:NZ	1:F:395:GLU:HG3	2.26	0.50
1:F:297:LEU:O	1:F:305:PHE:HA	2.11	0.50
1:A:10:PRO:CG	1:A:68:TYR:CD2	2.94	0.49
1:C:10:PRO:HG2	1:C:68:TYR:HD2	1.75	0.49
1:C:238:LYS:O	1:C:242:GLU:HG3	2.12	0.49
1:C:405:LEU:O	1:C:409:ILE:HG13	2.11	0.49
1:A:352:PRO:O	1:A:356:LYS:HG3	2.12	0.49
1:B:80:ASP:O	1:B:81:GLU:C	2.49	0.49
1:D:171:LYS:HE2	1:D:174:ASP:OD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:O	1:A:322:GLN:HG3	2.13	0.49
1:C:409:ILE:C	1:C:411:SER:H	2.14	0.49
1:F:35:TYR:CE2	1:F:409:ILE:HD12	2.46	0.49
1:A:50:ARG:CA	1:A:53:THR:HG22	2.42	0.49
1:D:213:THR:HG23	1:D:222:ASP:CB	2.35	0.49
1:D:5:ILE:HB	1:D:36:LEU:HD23	1.95	0.49
1:E:102:ASN:ND2	1:E:141:LYS:HG3	2.27	0.49
1:E:224:ARG:O	1:E:228:ILE:HG13	2.12	0.49
1:E:388:ARG:HD3	1:E:388:ARG:C	2.33	0.49
1:F:301:ASP:CB	1:F:303:LYS:HG2	2.42	0.49
1:B:133:ARG:HD2	1:B:277:ASP:N	2.27	0.49
1:B:50:ARG:HA	1:B:53:THR:HG22	1.92	0.49
1:C:151:GLY:HA3	1:D:159:PRO:HA	1.95	0.49
1:A:53:THR:HG21	1:A:57:ILE:CG2	2.40	0.49
1:C:274:TYR:O	1:C:278:VAL:HG23	2.13	0.49
1:C:350:ASN:O	1:C:352:PRO:HD2	2.13	0.49
1:F:127:LYS:HD3	1:F:266:GLY:HA3	1.94	0.49
1:D:134:HIS:HB2	1:D:194:PHE:CE1	2.47	0.49
1:D:203:ILE:HG23	1:D:244:LEU:CD1	2.42	0.49
1:D:351:THR:O	1:D:353:ALA:N	2.46	0.49
1:E:343:LEU:O	1:E:347:GLU:HG3	2.12	0.49
1:F:387:GLU:HG3	1:F:390:ALA:HB2	1.94	0.49
1:F:409:ILE:HG22	1:F:409:ILE:O	2.13	0.49
1:A:127:LYS:HD3	1:A:266:GLY:HA3	1.95	0.49
3:B:1201:NDP:HO3A	3:B:1201:NDP:P2B	2.36	0.49
1:B:293:MET:HG2	1:B:310:ALA:HB2	1.95	0.49
3:C:1301:NDP:H3B	3:C:1301:NDP:O3X	2.13	0.49
1:D:23:ILE:O	1:D:27:ILE:HG13	2.12	0.49
1:E:201:LEU:CD2	1:E:205:LYS:HG3	2.43	0.49
1:E:50:ARG:HA	1:E:53:THR:HG22	1.93	0.49
1:F:212:SER:OG	1:F:256:MET:HG2	2.13	0.49
1:A:203:ILE:HG23	1:A:244:LEU:CD1	2.42	0.49
1:A:170:LEU:HD11	1:B:145:THR:HG21	1.95	0.49
1:B:7:VAL:HB	1:B:38:VAL:HG12	1.95	0.49
1:F:72:ILE:HD13	1:F:338:TRP:HA	1.95	0.49
1:D:187:THR:O	1:D:191:ILE:HG13	2.13	0.48
1:F:240:LYS:HG3	5:F:1638:HOH:O	2.13	0.48
1:A:301:ASP:HB3	1:A:303:LYS:HG2	1.94	0.48
1:A:31:LEU:CD2	1:A:405:LEU:HD12	2.42	0.48
1:A:393:THR:HG23	1:A:396:GLU:OE2	2.13	0.48
1:B:249:GLU:OE1	1:B:251:ARG:NE	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ASP:OD1	1:D:46:SER:HA	2.13	0.48
1:D:131:ILE:HD13	1:D:269:MET:HB2	1.94	0.48
1:A:171:LYS:HE2	1:A:174:ASP:OD1	2.13	0.48
1:A:367:ASN:HB3	1:A:371:GLN:CG	2.44	0.48
1:C:336:PHE:CZ	1:C:362:GLU:HG2	2.49	0.48
1:F:17:ASP:CB	1:F:77:ILE:HG13	2.43	0.48
1:B:251:ARG:HD2	1:B:255:ASP:OD1	2.13	0.48
1:C:251:ARG:HD3	1:D:316:ARG:NH2	2.27	0.48
1:C:284:ALA:HB3	1:C:290:LEU:HD23	1.96	0.48
1:F:388:ARG:O	1:F:388:ARG:HD3	2.13	0.48
1:C:2:PHE:N	1:C:2:PHE:HD2	2.09	0.48
1:E:213:THR:CG2	1:E:215:ASN:HB3	2.43	0.48
1:E:117:ARG:HB2	1:E:370:GLN:OE1	2.14	0.48
1:F:224:ARG:HH12	1:F:228:ILE:CG1	2.26	0.48
1:E:187:THR:O	1:E:191:ILE:HG13	2.14	0.48
1:F:330:ASN:HD22	1:F:331:SER:N	2.11	0.48
1:A:319:ARG:HD3	1:A:322:GLN:HE21	1.77	0.48
1:E:183:ALA:HB2	1:F:155:LEU:HD23	1.96	0.48
1:F:292:LEU:HD11	1:F:379:LEU:CD2	2.43	0.48
1:A:121:LEU:C	1:A:123:PRO:HD3	2.34	0.48
1:A:129:ILE:HG13	1:A:287:PHE:CZ	2.48	0.48
1:E:316:ARG:HH22	1:F:251:ARG:CD	2.27	0.48
1:F:201:LEU:O	1:F:201:LEU:HD23	2.14	0.48
1:B:19:MET:HE1	1:B:318:TYR:HA	1.96	0.48
1:A:153:LEU:HD12	1:A:172:VAL:CB	2.44	0.47
1:B:121:LEU:C	1:B:123:PRO:HD3	2.34	0.47
1:B:405:LEU:HD13	1:B:409:ILE:HD11	1.96	0.47
1:B:55:ASP:HB2	1:B:93:TRP:CE3	2.49	0.47
1:C:178:SER:C	1:D:188:ASP:OD2	2.52	0.47
1:D:134:HIS:O	1:D:273:ASN:HA	2.13	0.47
1:D:9:GLN:OE1	1:D:9:GLN:HA	2.13	0.47
1:F:12:VAL:HG12	1:F:14:LEU:CD2	2.44	0.47
1:F:134:HIS:HB2	1:F:194:PHE:CE1	2.49	0.47
1:E:146:LEU:HD11	1:F:220:LYS:HB3	1.93	0.47
1:F:230:GLN:O	1:F:234:GLU:HG3	2.14	0.47
1:A:258:ALA:O	1:B:285:GLN:HG2	2.14	0.47
3:B:1201:NDP:O3B	3:B:1201:NDP:O1X	2.31	0.47
1:A:159:PRO:HA	1:B:151:GLY:HA3	1.96	0.47
1:E:111:GLU:HB3	1:E:130:ILE:HG12	1.96	0.47
1:E:175:TYR:OH	1:E:181:ALA:HB2	2.14	0.47
1:A:256:MET:HG3	1:A:269:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:OE2	1:C:28:LYS:NZ	2.35	0.47
1:D:188:ASP:O	1:D:192:GLU:HG3	2.13	0.47
1:E:2:PHE:CD2	1:E:2:PHE:N	2.81	0.47
1:E:191:ILE:HG21	1:E:228:ILE:HD12	1.96	0.47
1:F:292:LEU:HD11	1:F:379:LEU:HD21	1.95	0.47
1:C:156:VAL:HG11	1:C:158:LYS:HE3	1.96	0.47
1:C:175:TYR:OH	1:C:181:ALA:HB2	2.14	0.47
1:E:124:ARG:HB3	5:E:1530:HOH:O	2.14	0.47
1:C:116:PRO:HD2	1:C:370:GLN:HE21	1.79	0.47
1:C:127:LYS:HG2	1:C:266:GLY:HA2	1.97	0.47
1:D:210:PHE:CE2	1:D:251:ARG:NH2	2.82	0.47
1:E:221:TYR:HD1	1:F:182:MET:HB3	1.80	0.47
1:F:246:ILE:HG13	1:F:246:ILE:O	2.13	0.47
1:A:213:THR:HG23	1:A:222:ASP:CB	2.40	0.47
1:C:18:GLU:HB3	1:C:318:TYR:CG	2.49	0.47
1:D:161:ASP:C	1:D:163:THR:H	2.18	0.47
1:D:356:LYS:O	1:D:360:ILE:HG13	2.15	0.47
1:F:299:THR:OG1	1:F:304:THR:HB	2.14	0.47
1:A:134:HIS:HE1	1:A:186:ASN:OD1	1.96	0.47
1:C:76:THR:O	3:C:1301:NDP:H2N	2.14	0.47
1:A:24:TRP:CD2	1:A:74:CYS:HB2	2.49	0.47
1:A:92:MET:CE	1:B:219:LYS:HD3	2.44	0.47
1:F:121:LEU:O	1:F:123:PRO:HD3	2.14	0.47
1:F:213:THR:CG2	1:F:250:HIS:NE2	2.77	0.47
1:B:119:PRO:O	1:B:120:ARG:HG3	2.15	0.47
1:A:224:ARG:HD3	1:B:146:LEU:HD21	1.97	0.47
1:F:251:ARG:CD	1:F:255:ASP:OD1	2.62	0.47
1:D:116:PRO:HB2	1:D:370:GLN:HE22	1.80	0.47
1:C:146:LEU:HD12	1:D:220:LYS:HB3	1.97	0.47
1:A:108:VAL:HG23	1:A:135:ALA:HB2	1.97	0.46
1:A:140:TYR:CE1	1:A:274:TYR:HA	2.48	0.46
1:B:228:ILE:O	1:B:232:VAL:HG23	2.15	0.46
1:C:188:ASP:O	1:C:192:GLU:HG3	2.15	0.46
1:C:203:ILE:HG23	1:C:244:LEU:CD1	2.45	0.46
1:A:356:LYS:O	1:A:360:ILE:HG13	2.15	0.46
1:A:327:THR:CG2	1:A:394:THR:OG1	2.61	0.46
1:C:130:ILE:HB	1:C:268:ILE:HG12	1.96	0.46
1:E:29:LYS:O	1:E:34:PRO:HD3	2.15	0.46
1:A:161:ASP:C	1:A:163:THR:H	2.18	0.46
1:A:79:PRO:O	1:B:219:LYS:NZ	2.48	0.46
1:A:79:PRO:HG2	1:A:93:TRP:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:ASN:ND2	1:E:332:ILE:H	2.14	0.46
1:F:120:ARG:NH2	1:F:126:GLU:HA	2.30	0.46
3:B:1201:NDP:C4N	4:B:1202:AKG:C4	2.91	0.46
1:B:21:ARG:HH22	1:B:44:ASP:CG	2.18	0.46
1:D:109:PHE:CD1	1:D:201:LEU:CD1	2.98	0.46
1:D:106:GLY:O	1:D:135:ALA:HB3	2.15	0.46
1:E:111:GLU:HG3	5:E:1509:HOH:O	2.15	0.46
1:F:305:PHE:N	1:F:305:PHE:CD2	2.82	0.46
1:A:144:ASP:OD2	1:B:220:LYS:HB2	2.16	0.46
1:A:124:ARG:O	1:A:264:LYS:HA	2.15	0.46
1:A:79:PRO:HG3	1:A:93:TRP:HB2	1.97	0.46
1:C:318:TYR:O	1:C:322:GLN:HG3	2.16	0.46
1:E:172:VAL:O	1:E:173:TYR:HB2	2.16	0.46
1:A:117:ARG:HB2	1:A:370:GLN:OE1	2.15	0.46
1:A:402:GLU:O	1:A:406:GLN:HG3	2.16	0.46
1:D:8:LYS:HD3	1:D:349:ASP:HB3	1.97	0.46
1:E:116:PRO:HD2	1:E:370:GLN:NE2	2.31	0.46
1:F:36:LEU:CB	1:F:38:VAL:HG13	2.45	0.46
1:B:2:PHE:N	1:B:2:PHE:HD2	2.13	0.46
1:D:330:ASN:HD21	1:D:332:ILE:HD12	1.81	0.46
1:E:115:ILE:HG22	1:E:118:ILE:HG12	1.98	0.46
1:E:136:HIS:ND1	1:E:137:GLY:N	2.64	0.46
1:E:316:ARG:NH2	1:F:251:ARG:NE	2.64	0.46
1:E:285:GLN:HG2	1:F:258:ALA:O	2.16	0.46
1:B:201:LEU:HD22	1:B:268:ILE:HD11	1.97	0.46
1:C:219:LYS:NZ	1:D:79:PRO:O	2.47	0.46
1:D:29:LYS:O	1:D:34:PRO:CD	2.62	0.46
1:A:253:ILE:HG23	1:A:254:ASP:N	2.30	0.46
1:B:47:VAL:HG13	1:B:77:ILE:HB	1.97	0.46
1:C:212:SER:OG	1:C:256:MET:HG2	2.15	0.46
1:D:127:LYS:HD3	1:D:266:GLY:HA3	1.98	0.46
1:E:313:THR:C	1:E:314:VAL:HG23	2.35	0.46
1:A:116:PRO:CD	1:A:370:GLN:NE2	2.79	0.46
1:B:153:LEU:HD13	1:B:154:GLU:N	2.31	0.46
1:C:127:LYS:O	1:C:265:GLY:HA3	2.16	0.46
1:D:212:SER:OG	1:D:256:MET:HG2	2.16	0.46
1:E:241:PHE:CD2	1:E:246:ILE:HG13	2.51	0.46
1:F:211:LEU:HD23	1:F:212:SER:N	2.31	0.46
1:A:212:SER:OG	1:A:256:MET:HG2	2.16	0.45
1:A:238:LYS:O	1:A:242:GLU:HG3	2.17	0.45
1:B:14:LEU:N	1:B:14:LEU:HD23	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ALA:O	1:B:182:MET:HB3	2.15	0.45
1:B:191:ILE:O	1:B:194:PHE:HB3	2.16	0.45
1:B:332:ILE:O	1:B:336:PHE:HD1	1.99	0.45
1:B:395:GLU:OE1	1:B:395:GLU:N	2.47	0.45
1:E:248:TYR:CG	1:E:249:GLU:N	2.84	0.45
1:E:331:SER:O	1:E:335:ILE:HG13	2.17	0.45
1:F:26:LYS:NZ	1:F:395:GLU:CG	2.79	0.45
1:A:211:LEU:CD2	1:A:211:LEU:C	2.85	0.45
1:A:256:MET:HG3	1:A:269:MET:CE	2.46	0.45
1:B:153:LEU:HD12	1:B:172:VAL:HB	1.97	0.45
1:C:80:ASP:O	1:C:81:GLU:C	2.54	0.45
1:F:14:LEU:N	1:F:14:LEU:HD23	2.32	0.45
1:F:17:ASP:OD1	1:F:46:SER:HA	2.16	0.45
1:B:12:VAL:HG12	1:B:14:LEU:HD21	1.98	0.45
1:C:110:ARG:HG2	1:C:295:SER:HB2	1.98	0.45
1:E:147:ILE:HG13	1:E:175:TYR:CZ	2.50	0.45
1:A:321:TYR:HD1	5:A:1110:HOH:O	2.00	0.45
1:D:109:PHE:CE1	1:D:201:LEU:HD12	2.50	0.45
1:F:250:HIS:C	1:F:250:HIS:ND1	2.69	0.45
1:A:67:LYS:HD3	1:A:68:TYR:CE1	2.51	0.45
1:D:230:GLN:NE2	5:D:1431:HOH:O	2.49	0.45
1:E:45:LEU:O	1:E:50:ARG:NE	2.37	0.45
1:F:111:GLU:HB2	1:F:112:PRO:HD2	1.97	0.45
1:A:139:GLN:NE2	5:A:1119:HOH:O	2.48	0.45
1:B:79:PRO:HG3	1:B:93:TRP:HB2	1.98	0.45
1:C:367:ASN:HB3	1:C:371:GLN:HG3	1.97	0.45
1:C:79:PRO:O	1:D:219:LYS:NZ	2.50	0.45
1:D:161:ASP:O	1:D:163:THR:N	2.50	0.45
1:E:19:MET:HE3	1:E:327:THR:HG21	1.99	0.45
1:F:327:THR:HG22	1:F:328:SER:H	1.82	0.45
1:A:161:ASP:O	1:A:163:THR:N	2.49	0.45
1:E:127:LYS:HD3	1:E:266:GLY:CA	2.45	0.45
3:F:1601:NDP:O3B	3:F:1601:NDP:O1X	2.35	0.45
1:F:211:LEU:HD12	1:F:229:PHE:CG	2.52	0.45
1:A:180:VAL:HG23	1:B:221:TYR:CE1	2.52	0.45
1:C:342:LEU:HB3	1:C:354:LEU:HD22	1.98	0.45
1:C:316:ARG:NH2	1:D:255:ASP:OD1	2.50	0.45
1:E:401:VAL:O	1:E:405:LEU:HB2	2.17	0.45
1:F:147:ILE:N	1:F:179:GLY:O	2.44	0.45
1:B:23:ILE:O	1:B:27:ILE:HG13	2.17	0.45
1:E:133:ARG:CZ	1:E:277:ASP:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:THR:HG23	1:C:214:LYS:N	2.32	0.45
1:E:219:LYS:HD3	1:F:92:MET:CE	2.46	0.45
1:F:326:GLU:CD	1:F:388:ARG:HH21	2.20	0.45
1:F:374:ILE:HG23	1:F:392:VAL:HG11	1.99	0.45
1:A:312:GLY:N	3:A:1101:NDP:O1A	2.41	0.44
1:A:247:HIS:ND1	1:A:247:HIS:N	2.65	0.44
1:B:368:THR:HG22	1:B:374:ILE:HB	1.99	0.44
1:C:213:THR:HG21	1:C:222:ASP:HB3	1.97	0.44
1:C:404:ARG:NH1	1:C:408:GLU:OE2	2.49	0.44
1:B:120:ARG:CZ	1:B:125:TRP:O	2.65	0.44
1:C:319:ARG:HD3	1:C:322:GLN:NE2	2.30	0.44
1:F:24:TRP:CD2	1:F:74:CYS:HB2	2.52	0.44
1:F:301:ASP:HB3	1:F:303:LYS:CG	2.46	0.44
1:C:288:GLY:O	1:C:289:SER:HB3	2.16	0.44
1:D:125:TRP:CZ3	1:D:286:GLY:HA3	2.52	0.44
1:F:24:TRP:HH2	1:F:72:ILE:HG22	1.82	0.44
1:A:291:GLY:O	1:A:333:ALA:HB2	2.18	0.44
1:C:129:ILE:HG13	1:C:287:PHE:HZ	1.82	0.44
1:C:216:THR:HB	1:D:78:THR:HG21	1.99	0.44
1:E:212:SER:HB3	1:E:253:ILE:HA	1.99	0.44
1:E:54:SER:HA	1:E:93:TRP:CH2	2.52	0.44
1:F:108:VAL:HG23	1:F:135:ALA:HB2	1.99	0.44
1:C:152:SER:O	1:D:157:TYR:HD1	2.00	0.44
1:C:201:LEU:HD21	1:C:205:LYS:HD2	2.00	0.44
1:C:22:ILE:CD1	1:C:321:TYR:CE2	3.00	0.44
1:D:393:THR:H	1:D:396:GLU:HB2	1.82	0.44
1:D:57:ILE:HG23	1:D:58:THR:N	2.33	0.44
1:E:320:LYS:O	1:E:325:GLU:HB2	2.17	0.44
1:A:73:LYS:HG2	1:A:74:CYS:O	2.17	0.44
1:B:24:TRP:HH2	1:B:72:ILE:HG22	1.82	0.44
1:C:109:PHE:CD1	1:C:201:LEU:HD12	2.53	0.44
1:D:21:ARG:NH2	1:D:44:ASP:OD1	2.50	0.44
1:E:202:ALA:CA	1:E:268:ILE:HD12	2.44	0.44
1:B:393:THR:OG1	1:B:396:GLU:HG3	2.17	0.44
1:C:108:VAL:CG2	1:C:135:ALA:HB2	2.47	0.44
1:C:171:LYS:HE2	1:C:174:ASP:CG	2.38	0.44
1:C:179:GLY:N	1:D:188:ASP:OD2	2.50	0.44
1:C:308:GLU:HG3	1:C:309:ALA:O	2.17	0.44
1:C:220:LYS:HB2	1:D:144:ASP:OD2	2.17	0.44
1:D:109:PHE:CD1	1:D:201:LEU:HD12	2.52	0.44
1:E:195:ALA:HA	1:E:229:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:TRP:CE3	1:F:74:CYS:HB2	2.53	0.44
1:A:10:PRO:CG	1:A:68:TYR:HD2	2.31	0.44
1:B:173:TYR:CG	1:B:174:ASP:N	2.86	0.44
1:B:251:ARG:CG	1:B:251:ARG:HH11	2.31	0.44
1:C:22:ILE:HD11	1:C:321:TYR:CE2	2.53	0.44
1:E:299:THR:OG1	1:E:304:THR:HB	2.17	0.44
1:E:56:LYS:HB3	5:E:1526:HOH:O	2.16	0.44
1:E:96:PRO:O	1:E:100:ILE:HG13	2.18	0.44
1:F:326:GLU:OE1	1:F:388:ARG:NH2	2.50	0.44
1:A:365:THR:HA	1:A:401:VAL:HG13	1.99	0.44
1:C:4:LYS:HE2	1:C:34:PRO:O	2.18	0.44
1:D:147:ILE:HG13	1:D:175:TYR:CZ	2.53	0.44
1:D:210:PHE:CE2	1:D:251:ARG:CZ	3.00	0.44
1:D:47:VAL:O	1:D:51:ASP:N	2.44	0.44
1:E:76:THR:O	3:E:1501:NDP:H2N	2.18	0.44
1:F:377:LYS:HG3	1:F:391:TYR:CE2	2.53	0.44
1:A:213:THR:HB	1:A:250:HIS:NE2	2.33	0.43
1:C:171:LYS:CE	1:C:174:ASP:OD1	2.64	0.43
1:C:61:ALA:O	1:C:65:ILE:HG13	2.18	0.43
1:D:120:ARG:CZ	1:D:126:GLU:HA	2.48	0.43
1:D:120:ARG:NH1	1:D:126:GLU:HA	2.33	0.43
1:D:283:VAL:O	1:D:287:PHE:HD1	2.00	0.43
1:D:28:LYS:NZ	5:D:1433:HOH:O	2.50	0.43
1:E:403:LYS:HG2	1:E:407:LYS:HE2	1.99	0.43
1:F:188:ASP:O	1:F:192:GLU:HG3	2.17	0.43
1:A:171:LYS:HE2	1:A:174:ASP:OD2	2.19	0.43
1:A:297:LEU:HB3	1:A:306:GLU:HB3	1.99	0.43
1:A:50:ARG:O	1:A:53:THR:HG22	2.18	0.43
1:B:153:LEU:HB2	1:B:175:TYR:HE1	1.83	0.43
1:C:327:THR:HG22	1:C:328:SER:N	2.32	0.43
1:E:41:LYS:O	1:E:43:TYR:HD1	2.02	0.43
1:A:327:THR:HG22	1:A:328:SER:N	2.33	0.43
3:B:1201:NDP:C5N	4:B:1202:AKG:H42	2.48	0.43
1:A:224:ARG:HD3	1:B:146:LEU:CD2	2.48	0.43
1:B:24:TRP:O	1:B:27:ILE:HB	2.18	0.43
1:B:212:SER:OG	1:B:256:MET:HG2	2.18	0.43
1:C:14:LEU:N	1:C:14:LEU:CD2	2.81	0.43
1:D:14:LEU:N	1:D:14:LEU:HD23	2.33	0.43
1:F:134:HIS:O	1:F:273:ASN:HA	2.17	0.43
1:F:213:THR:HG22	1:F:250:HIS:NE2	2.33	0.43
1:F:96:PRO:O	1:F:100:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:HE2	1:B:219:LYS:HD3	2.01	0.43
1:B:51:ASP:HB2	1:B:89:LEU:HD22	2.00	0.43
1:C:213:THR:CG2	1:C:215:ASN:N	2.80	0.43
1:D:118:ILE:HA	1:D:119:PRO:HD3	1.72	0.43
3:D:1401:NDP:C5N	4:D:1402:AKG:H42	2.47	0.43
1:E:171:LYS:HE2	1:E:174:ASP:OD2	2.18	0.43
1:E:196:HIS:CE1	1:E:232:VAL:HG13	2.53	0.43
1:E:405:LEU:CD2	1:E:409:ILE:HD11	2.46	0.43
1:F:169:THR:HG22	1:F:169:THR:O	2.18	0.43
1:F:340:ARG:HA	1:F:340:ARG:HD3	1.83	0.43
1:C:121:LEU:C	1:C:123:PRO:HD3	2.38	0.43
3:C:1301:NDP:C4N	4:C:1302:AKG:C4	2.88	0.43
1:A:221:TYR:CE1	1:B:182:MET:HG2	2.53	0.43
1:B:209:LEU:HD23	1:B:210:PHE:N	2.33	0.43
3:C:1301:NDP:C3N	4:C:1302:AKG:H41	2.49	0.43
1:D:233:TYR:CZ	1:D:238:LYS:HA	2.54	0.43
1:F:109:PHE:CZ	1:F:201:LEU:HD12	2.54	0.43
1:E:157:TYR:OH	1:F:149:GLY:O	2.30	0.43
1:F:327:THR:CG2	1:F:328:SER:N	2.82	0.43
1:A:388:ARG:HD3	1:A:388:ARG:O	2.19	0.43
1:A:220:LYS:CD	1:B:145:THR:HA	2.49	0.43
1:D:213:THR:HG21	1:D:222:ASP:HB3	2.00	0.43
1:D:409:ILE:C	1:D:411:SER:N	2.72	0.43
1:A:7:VAL:HG21	1:A:38:VAL:CG1	2.48	0.43
1:B:192:GLU:HG2	1:B:228:ILE:HG21	2.00	0.43
1:E:10:PRO:HG2	1:E:68:TYR:CE2	2.53	0.43
1:E:16:GLY:HA3	1:E:75:ALA:O	2.19	0.43
1:E:109:PHE:CD1	1:E:201:LEU:HD12	2.53	0.43
1:E:97:ASN:HD21	3:E:1501:NDP:C7N	2.31	0.43
1:F:344:LYS:HA	1:F:344:LYS:HD3	1.82	0.43
1:F:372:ASP:CG	1:F:404:ARG:HE	2.22	0.43
1:E:216:THR:HG22	1:F:80:ASP:HB3	2.00	0.43
3:B:1201:NDP:C4N	4:B:1202:AKG:H41	2.47	0.43
1:B:119:PRO:C	1:B:120:ARG:HG3	2.39	0.43
1:B:187:THR:O	1:B:191:ILE:HG13	2.18	0.43
1:C:143:THR:O	1:C:182:MET:HA	2.19	0.43
1:E:44:ASP:O	1:E:57:ILE:HD13	2.18	0.43
1:F:35:TYR:CE1	1:F:405:LEU:HD13	2.54	0.43
3:A:1101:NDP:C3N	4:A:1102:AKG:H41	2.49	0.43
1:A:282:ILE:HD13	1:B:282:ILE:HD13	2.01	0.43
1:A:343:LEU:HG	1:A:358:ALA:HB1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:GLU:CD	1:E:388:ARG:HH21	2.22	0.43
1:A:39:ASP:OD2	1:A:41:LYS:HE2	2.19	0.42
1:B:133:ARG:HB2	1:B:276:GLY:HA3	2.00	0.42
1:B:192:GLU:HG2	1:B:228:ILE:CG2	2.49	0.42
1:B:213:THR:HG23	1:B:222:ASP:CB	2.45	0.42
1:C:10:PRO:CG	1:C:68:TYR:CD2	3.00	0.42
1:E:296:ILE:HG23	1:E:296:ILE:O	2.18	0.42
1:A:256:MET:HE3	1:A:259:GLN:HB2	2.01	0.42
1:E:393:THR:OG1	1:E:396:GLU:HG3	2.19	0.42
1:F:117:ARG:NH1	1:F:370:GLN:O	2.52	0.42
1:F:402:GLU:OE2	5:F:1621:HOH:O	2.22	0.42
1:A:250:HIS:C	1:A:250:HIS:ND1	2.73	0.42
1:A:96:PRO:HA	5:A:1109:HOH:O	2.19	0.42
1:C:21:ARG:NH2	1:C:44:ASP:CG	2.73	0.42
1:C:397:PHE:O	1:C:401:VAL:HG23	2.19	0.42
1:E:316:ARG:NH2	1:F:251:ARG:CD	2.83	0.42
1:E:388:ARG:C	1:E:390:ALA:H	2.22	0.42
1:F:403:LYS:HB3	1:F:403:LYS:NZ	2.33	0.42
1:A:38:VAL:HG23	1:A:40:LEU:HG	2.01	0.42
1:B:164:THR:HG22	1:B:164:THR:O	2.20	0.42
1:F:345:ARG:HA	1:F:345:ARG:NE	2.33	0.42
1:F:35:TYR:CZ	1:F:405:LEU:HD13	2.55	0.42
1:B:147:ILE:HA	1:B:148:PRO:HD2	1.81	0.42
1:C:17:ASP:CB	1:C:77:ILE:HG13	2.49	0.42
1:D:121:LEU:O	1:D:123:PRO:HD3	2.19	0.42
1:E:253:ILE:HG23	1:E:254:ASP:N	2.34	0.42
1:F:153:LEU:HD12	1:F:172:VAL:CG1	2.50	0.42
1:A:319:ARG:HA	1:A:322:GLN:HE21	1.84	0.42
3:D:1401:NDP:C4N	4:D:1402:AKG:C4	2.95	0.42
1:D:248:TYR:CG	1:D:249:GLU:N	2.87	0.42
1:D:10:PRO:HG2	1:D:68:TYR:CD2	2.54	0.42
1:F:127:LYS:HG2	1:F:266:GLY:HA2	2.02	0.42
1:F:10:PRO:CG	1:F:68:TYR:CD2	2.97	0.42
1:B:120:ARG:NH2	1:B:287:PHE:CE2	2.88	0.42
1:B:343:LEU:O	1:B:347:GLU:HG3	2.20	0.42
1:C:125:TRP:HZ3	1:C:286:GLY:HA3	1.84	0.42
1:C:139:GLN:HB3	1:C:184:MET:HE2	2.01	0.42
1:C:327:THR:CG2	1:C:328:SER:N	2.82	0.42
1:C:221:TYR:N	1:D:144:ASP:OD2	2.47	0.42
1:D:53:THR:HG21	1:D:57:ILE:CG2	2.50	0.42
1:D:96:PRO:O	1:D:100:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:O	1:A:293:MET:HG3	2.20	0.42
1:D:157:TYR:HB3	1:D:168:GLN:HB2	2.01	0.42
1:E:155:LEU:HD23	1:F:183:ALA:HB2	2.02	0.42
1:E:19:MET:HB3	1:E:313:THR:O	2.18	0.42
1:E:87:PHE:HB2	1:E:89:LEU:CD2	2.49	0.42
1:F:247:HIS:ND1	1:F:247:HIS:N	2.68	0.42
1:F:248:TYR:CG	1:F:249:GLU:N	2.88	0.42
1:F:270:ALA:O	1:F:271:LEU:HD23	2.20	0.42
1:A:251:ARG:HD2	1:A:255:ASP:OD1	2.19	0.42
1:A:349:ASP:O	1:A:350:ASN:C	2.58	0.42
1:B:24:TRP:CH2	1:B:72:ILE:HG22	2.55	0.42
1:E:173:TYR:CG	1:E:174:ASP:N	2.88	0.42
1:E:221:TYR:CD1	1:F:182:MET:HB3	2.55	0.42
1:F:140:TYR:HE1	1:F:274:TYR:HA	1.85	0.42
1:A:367:ASN:HB3	1:A:371:GLN:HG2	2.01	0.42
1:B:119:PRO:HG2	1:B:383:CYS:HA	2.01	0.42
1:D:19:MET:HE2	1:D:318:TYR:N	2.35	0.42
1:E:36:LEU:CB	1:E:38:VAL:HG13	2.50	0.42
1:F:148:PRO:O	1:F:178:SER:HB3	2.20	0.42
1:F:310:ALA:HB3	5:F:1607:HOH:O	2.19	0.42
1:B:8:LYS:CD	1:B:349:ASP:HB3	2.50	0.41
1:C:248:TYR:O	1:C:249:GLU:HB2	2.19	0.41
1:D:13:GLU:OE1	1:D:40:LEU:HD13	2.20	0.41
1:E:108:VAL:HG23	1:E:135:ALA:HB2	2.02	0.41
1:F:240:LYS:O	1:F:243:GLN:HB3	2.19	0.41
1:F:90:HIS:CD2	1:F:91:LYS:HG3	2.54	0.41
1:B:160:SER:O	1:B:162:PRO:HD3	2.20	0.41
1:F:253:ILE:O	1:F:257:VAL:HG13	2.19	0.41
1:A:121:LEU:HD13	1:B:262:LYS:HA	2.02	0.41
1:F:133:ARG:CZ	1:F:277:ASP:HB2	2.51	0.41
1:B:19:MET:HE2	1:B:317:HIS:C	2.40	0.41
1:B:338:TRP:O	1:B:342:LEU:HG	2.20	0.41
1:C:161:ASP:C	1:C:163:THR:H	2.23	0.41
1:C:5:ILE:HD12	1:C:357:PHE:HB2	2.02	0.41
1:E:153:LEU:HD13	1:E:154:GLU:N	2.35	0.41
1:F:263:SER:HB2	5:F:1619:HOH:O	2.19	0.41
1:F:318:TYR:O	1:F:321:TYR:HB3	2.20	0.41
1:A:125:TRP:CZ3	1:A:286:GLY:HA3	2.47	0.41
1:A:313:THR:C	1:A:314:VAL:HG23	2.40	0.41
1:C:121:LEU:O	1:C:123:PRO:HD3	2.20	0.41
1:D:211:LEU:HD13	1:D:250:HIS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LEU:HB3	1:E:267:PHE:HA	2.03	0.41
1:E:403:LYS:HA	1:E:406:GLN:OE1	2.19	0.41
1:A:122:VAL:HB	1:A:125:TRP:CE3	2.55	0.41
1:A:111:GLU:HB3	1:A:130:ILE:HG12	2.03	0.41
1:B:140:TYR:CD1	1:B:140:TYR:N	2.88	0.41
1:D:137:GLY:O	1:D:138:ASP:C	2.57	0.41
3:D:1401:NDP:O3B	3:D:1401:NDP:O1X	2.38	0.41
1:D:340:ARG:HA	1:D:340:ARG:HD3	1.90	0.41
1:E:409:ILE:C	1:E:411:SER:N	2.72	0.41
1:E:8:LYS:HB3	1:E:349:ASP:CB	2.49	0.41
1:F:402:GLU:O	1:F:406:GLN:HG3	2.20	0.41
1:A:315:THR:O	1:A:319:ARG:HG2	2.21	0.41
1:A:296:ILE:CD1	1:A:344:LYS:HG3	2.49	0.41
1:E:118:ILE:HA	1:E:119:PRO:HD3	1.80	0.41
1:E:316:ARG:NH2	1:F:251:ARG:HD3	2.35	0.41
1:B:299:THR:CG2	1:B:304:THR:HB	2.50	0.41
1:B:79:PRO:CG	1:B:93:TRP:O	2.67	0.41
1:C:263:SER:HG	1:C:267:PHE:HE2	1.69	0.41
1:C:146:LEU:CD1	1:D:220:LYS:HB3	2.50	0.41
1:D:28:LYS:O	1:D:33:LEU:HG	2.20	0.41
1:E:36:LEU:HD21	1:E:357:PHE:CD2	2.56	0.41
1:A:340:ARG:HD3	1:A:340:ARG:HA	1.85	0.41
1:A:50:ARG:C	1:A:53:THR:HG22	2.41	0.41
1:B:124:ARG:HB2	5:B:1224:HOH:O	2.21	0.41
1:A:316:ARG:NH2	1:B:251:ARG:NE	2.68	0.41
1:C:351:THR:O	1:C:353:ALA:N	2.54	0.41
1:A:171:LYS:HE2	1:A:174:ASP:CG	2.41	0.41
1:B:67:LYS:HD3	1:B:68:TYR:CZ	2.56	0.41
1:C:105:GLY:O	1:C:297:LEU:HD11	2.21	0.41
1:D:45:LEU:O	1:D:50:ARG:NE	2.53	0.41
1:D:57:ILE:CG2	1:D:58:THR:N	2.84	0.41
1:A:101:ARG:HD2	5:A:1115:HOH:O	2.21	0.41
1:A:59:GLN:NE2	1:A:103:ILE:HD11	2.36	0.41
1:A:12:VAL:HG12	1:A:14:LEU:CD2	2.50	0.41
1:A:54:SER:HA	1:A:93:TRP:CH2	2.55	0.41
1:B:367:ASN:CB	1:B:371:GLN:HG3	2.45	0.41
1:C:136:HIS:CG	1:C:137:GLY:N	2.86	0.41
1:D:409:ILE:C	1:D:411:SER:H	2.25	0.41
1:A:158:LYS:HA	1:A:159:PRO:HD2	1.98	0.40
1:A:336:PHE:HA	1:A:339:SER:OG	2.21	0.40
1:B:19:MET:CE	1:B:318:TYR:HA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASP:O	1:B:82:ALA:N	2.55	0.40
1:C:45:LEU:HD22	1:C:57:ILE:HG23	2.02	0.40
1:C:72:ILE:HD13	1:C:338:TRP:HA	2.03	0.40
1:D:134:HIS:HE1	1:D:186:ASN:OD1	2.04	0.40
1:C:251:ARG:HD2	1:C:255:ASP:OD1	2.20	0.40
1:D:138:ASP:HB3	1:D:139:GLN:OE1	2.22	0.40
1:A:119:PRO:C	1:A:120:ARG:HG3	2.41	0.40
1:B:284:ALA:HB3	1:B:290:LEU:HD23	2.04	0.40
1:E:137:GLY:O	1:E:138:ASP:HB2	2.21	0.40
1:F:195:ALA:HA	1:F:229:PHE:CE2	2.57	0.40
3:A:1101:NDP:O3B	3:A:1101:NDP:O1X	2.39	0.40
1:A:134:HIS:CD2	1:A:194:PHE:HB2	2.57	0.40
1:A:330:ASN:HD22	1:A:331:SER:N	2.19	0.40
3:B:1201:NDP:O3B	3:B:1201:NDP:O3X	2.37	0.40
1:B:148:PRO:O	1:B:178:SER:HB3	2.21	0.40
1:C:145:THR:HA	1:D:220:LYS:HD2	2.02	0.40
1:C:67:LYS:HD3	1:C:68:TYR:CE1	2.56	0.40
1:A:401:VAL:O	1:A:405:LEU:HB2	2.22	0.40
1:B:112:PRO:HA	1:B:292:LEU:O	2.22	0.40
1:B:311:HIS:CD2	3:B:1201:NDP:H61A	2.40	0.40
1:B:12:VAL:HG12	1:B:14:LEU:CD2	2.51	0.40
1:B:17:ASP:HB2	1:B:77:ILE:HG13	2.03	0.40
1:D:43:TYR:OH	1:D:64:ALA:HB2	2.21	0.40
1:D:50:ARG:HA	1:D:53:THR:HG22	2.03	0.40
3:E:1501:NDP:C3N	4:E:1502:AKG:H42	2.51	0.40
1:E:232:VAL:HG12	1:E:237:TYR:HE1	1.86	0.40
1:E:392:VAL:HB	1:E:396:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/427 (96%)	365 (90%)	35 (9%)	8 (2%)	7	19
1	B	408/427 (96%)	368 (90%)	32 (8%)	8 (2%)	7	19
1	C	408/427 (96%)	364 (89%)	35 (9%)	9 (2%)	6	17
1	D	408/427 (96%)	359 (88%)	43 (10%)	6 (2%)	10	26
1	E	408/427 (96%)	364 (89%)	39 (10%)	5 (1%)	13	32
1	F	408/427 (96%)	361 (88%)	41 (10%)	6 (2%)	10	26
All	All	2448/2562 (96%)	2181 (89%)	225 (9%)	42 (2%)	9	23

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	236	GLN
1	B	8	LYS
1	D	8	LYS
1	E	8	LYS
1	E	141	LYS
1	A	18	GLU
1	B	81	GLU
1	B	141	LYS
1	B	324	GLY
1	C	8	LYS
1	C	136	HIS
1	A	141	LYS
1	A	162	PRO
1	A	249	GLU
1	C	139	GLN
1	C	167	PRO
1	F	141	LYS
1	A	408	GLU
1	B	162	PRO
1	C	162	PRO
1	C	215	ASN
1	D	18	GLU
1	D	162	PRO
1	D	236	GLN
1	F	8	LYS
1	F	408	GLU
1	A	407	LYS
1	C	410	LYS
1	D	167	PRO

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Mol	Chain	Res	Type
1	E	138	ASP
1	E	296	ILE
1	F	162	PRO
1	B	150	PRO
1	B	284	ALA
1	C	352	PRO
1	D	352	PRO
1	F	18	GLU
1	E	162	PRO
1	F	167	PRO
1	B	148	PRO
1	C	351	THR

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	354/367 (96%)	332 (94%)	22 (6%)	18	40
1	B	354/367 (96%)	332 (94%)	22 (6%)	18	40
1	C	354/367 (96%)	332 (94%)	22 (6%)	18	40
1	D	354/367 (96%)	331 (94%)	23 (6%)	17	38
1	E	354/367 (96%)	330 (93%)	24 (7%)	16	36
1	F	354/367 (96%)	330 (93%)	24 (7%)	16	36
All	All	2124/2202 (96%)	1987 (94%)	137 (6%)	17	38

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PHE
1	A	47	VAL
1	A	116	PRO
1	A	139	GLN
1	A	201	LEU
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	211	LEU
1	A	213	THR
1	A	218	LEU
1	A	229	PHE
1	A	247	HIS
1	A	251	ARG
1	A	254	ASP
1	A	301	ASP
1	A	314	VAL
1	A	330	ASN
1	A	331	SER
1	A	350	ASN
1	A	354	LEU
1	A	361	LEU
1	A	388	ARG
1	A	405	LEU
1	B	2	PHE
1	B	47	VAL
1	B	95	SER
1	B	139	GLN
1	B	153	LEU
1	B	209	LEU
1	B	211	LEU
1	B	218	LEU
1	B	236	GLN
1	B	247	HIS
1	B	251	ARG
1	B	254	ASP
1	B	297	LEU
1	B	301	ASP
1	B	314	VAL
1	B	330	ASN
1	B	331	SER
1	B	354	LEU
1	B	361	LEU
1	B	372	ASP
1	B	388	ARG
1	B	405	LEU
1	C	2	PHE
1	C	14	LEU
1	C	21	ARG
1	C	47	VAL

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Mol	Chain	Res	Type
1	C	95	SER
1	C	139	GLN
1	C	152	SER
1	C	153	LEU
1	C	209	LEU
1	C	211	LEU
1	C	218	LEU
1	C	229	PHE
1	C	251	ARG
1	C	330	ASN
1	C	331	SER
1	C	343	LEU
1	C	350	ASN
1	C	354	LEU
1	C	361	LEU
1	C	372	ASP
1	C	388	ARG
1	C	405	LEU
1	D	2	PHE
1	D	14	LEU
1	D	47	VAL
1	D	95	SER
1	D	120	ARG
1	D	139	GLN
1	D	152	SER
1	D	153	LEU
1	D	209	LEU
1	D	211	LEU
1	D	218	LEU
1	D	247	HIS
1	D	251	ARG
1	D	297	LEU
1	D	301	ASP
1	D	305	PHE
1	D	330	ASN
1	D	343	LEU
1	D	354	LEU
1	D	361	LEU
1	D	376	THR
1	D	388	ARG
1	D	405	LEU
1	E	2	PHE

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Mol	Chain	Res	Type
1	E	47	VAL
1	E	80	ASP
1	E	88	ASN
1	E	139	GLN
1	E	182	MET
1	E	186	ASN
1	E	201	LEU
1	E	209	LEU
1	E	211	LEU
1	E	213	THR
1	E	218	LEU
1	E	239	SER
1	E	247	HIS
1	E	254	ASP
1	E	314	VAL
1	E	330	ASN
1	E	331	SER
1	E	354	LEU
1	E	361	LEU
1	E	372	ASP
1	E	388	ARG
1	E	404	ARG
1	E	405	LEU
1	F	2	PHE
1	F	47	VAL
1	F	55	ASP
1	F	95	SER
1	F	120	ARG
1	F	155	LEU
1	F	161	ASP
1	F	186	ASN
1	F	209	LEU
1	F	211	LEU
1	F	213	THR
1	F	218	LEU
1	F	247	HIS
1	F	251	ARG
1	F	305	PHE
1	F	314	VAL
1	F	330	ASN
1	F	331	SER
1	F	354	LEU

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Mol	Chain	Res	Type
1	F	361	LEU
1	F	376	THR
1	F	388	ARG
1	F	403	LYS
1	F	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	88	ASN
1	A	90	HIS
1	A	97	ASN
1	A	102	ASN
1	A	322	GLN
1	A	330	ASN
1	A	359	ASN
1	B	88	ASN
1	B	102	ASN
1	B	322	GLN
1	B	330	ASN
1	B	370	GLN
1	C	59	GLN
1	C	88	ASN
1	C	90	HIS
1	C	102	ASN
1	C	259	GLN
1	C	322	GLN
1	C	330	ASN
1	C	359	ASN
1	C	370	GLN
1	C	386	ASN
1	D	90	HIS
1	D	136	HIS
1	D	259	GLN
1	D	322	GLN
1	D	330	ASN
1	D	370	GLN
1	E	59	GLN
1	E	102	ASN
1	E	259	GLN
1	E	322	GLN

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Mol	Chain	Res	Type
1	E	330	ASN
1	E	359	ASN
1	F	90	HIS
1	F	230	GLN
1	F	236	GLN
1	F	259	GLN
1	F	322	GLN
1	F	330	ASN
1	F	370	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 ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
3	NDP	C	1301	-	45,52,52	1.27	5 (11%)	53,80,80	1.02	2 (3%)
3	NDP	B	1201	-	45,52,52	1.28	5 (11%)	53,80,80	0.99	2 (3%)
4	AKG	E	1502	-	3,9,9	1.00	0	4,11,11	0.98	0
4	AKG	D	1402	-	3,9,9	1.05	0	4,11,11	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AKG	B	1202	-	3,9,9	1.07	0	4,11,11	0.71	0
4	AKG	A	1102	-	3,9,9	1.08	0	4,11,11	0.69	0
3	NDP	F	1601	-	45,52,52	1.27	5 (11%)	53,80,80	1.09	3 (5%)
3	NDP	D	1401	-	45,52,52	1.27	5 (11%)	53,80,80	1.09	3 (5%)
4	AKG	C	1302	-	3,9,9	1.02	0	4,11,11	0.92	0
3	NDP	E	1501	-	45,52,52	1.28	5 (11%)	53,80,80	1.11	3 (5%)
3	NDP	A	1101	-	45,52,52	1.27	5 (11%)	53,80,80	1.02	4 (7%)
4	AKG	F	1602	-	3,9,9	1.05	0	4,11,11	0.55	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
3	NDP	C	1301	-	-	12/30/77/77	0/5/5/5
3	NDP	B	1201	-	-	12/30/77/77	0/5/5/5
4	AKG	E	1502	-	-	1/3/9/9	-
4	AKG	D	1402	-	-	2/3/9/9	-
4	AKG	B	1202	-	-	2/3/9/9	-
4	AKG	A	1102	-	-	2/3/9/9	-
3	NDP	F	1601	-	-	13/30/77/77	0/5/5/5
3	NDP	D	1401	-	-	12/30/77/77	0/5/5/5
4	AKG	C	1302	-	-	2/3/9/9	-
3	NDP	E	1501	-	-	10/30/77/77	0/5/5/5
3	NDP	A	1101	-	-	13/30/77/77	0/5/5/5
4	AKG	F	1602	-	-	0/3/9/9	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	NDP	C4N-C5N	-3.64	1.39	1.48
3	C	1301	NDP	C4N-C5N	-3.57	1.39	1.48
3	D	1401	NDP	C4N-C5N	-3.55	1.39	1.48
3	A	1101	NDP	C4N-C5N	-3.54	1.39	1.48
3	E	1501	NDP	C4N-C5N	-3.54	1.39	1.48
3	F	1601	NDP	C4N-C5N	-3.52	1.39	1.48
3	B	1201	NDP	C6N-C5N	3.46	1.39	1.33
3	D	1401	NDP	C6N-C5N	3.43	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1501	NDP	C6N-C5N	3.40	1.39	1.33
3	C	1301	NDP	C6N-C5N	3.38	1.39	1.33
3	A	1101	NDP	C6N-C5N	3.36	1.39	1.33
3	F	1601	NDP	C6N-C5N	3.36	1.39	1.33
3	C	1301	NDP	PN-O1N	2.99	1.61	1.50
3	F	1601	NDP	PN-O1N	2.98	1.61	1.50
3	E	1501	NDP	PN-O1N	2.98	1.61	1.50
3	B	1201	NDP	PN-O1N	2.96	1.61	1.50
3	A	1101	NDP	PN-O1N	2.93	1.61	1.50
3	D	1401	NDP	PN-O1N	2.91	1.61	1.50
3	F	1601	NDP	O4B-C1B	2.38	1.44	1.41
3	E	1501	NDP	O4B-C1B	2.33	1.44	1.41
3	D	1401	NDP	O4B-C1B	2.30	1.44	1.41
3	A	1101	NDP	O4B-C1B	2.29	1.44	1.41
3	B	1201	NDP	O4B-C1B	2.28	1.44	1.41
3	B	1201	NDP	C7N-C3N	2.22	1.53	1.48
3	C	1301	NDP	O4B-C1B	2.22	1.44	1.41
3	C	1301	NDP	C7N-C3N	2.21	1.53	1.48
3	D	1401	NDP	C7N-C3N	2.19	1.53	1.48
3	F	1601	NDP	C7N-C3N	2.16	1.53	1.48
3	E	1501	NDP	C7N-C3N	2.15	1.53	1.48
3	A	1101	NDP	C7N-C3N	2.12	1.53	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1501	NDP	N3A-C2A-N1A	-4.54	121.58	128.68
3	B	1201	NDP	N3A-C2A-N1A	-4.38	121.84	128.68
3	D	1401	NDP	N3A-C2A-N1A	-4.37	121.86	128.68
3	C	1301	NDP	N3A-C2A-N1A	-4.34	121.89	128.68
3	A	1101	NDP	N3A-C2A-N1A	-4.26	122.02	128.68
3	F	1601	NDP	N3A-C2A-N1A	-4.24	122.05	128.68
3	E	1501	NDP	PN-O3-PA	-3.50	120.82	132.83
3	D	1401	NDP	PN-O3-PA	-3.27	121.60	132.83
3	C	1301	NDP	PN-O3-PA	-2.95	122.69	132.83
3	F	1601	NDP	PN-O3-PA	-2.83	123.11	132.83
3	A	1101	NDP	PN-O3-PA	-2.82	123.15	132.83
3	B	1201	NDP	PN-O3-PA	-2.57	124.00	132.83
3	D	1401	NDP	C3N-C2N-N1N	-2.19	119.97	123.10
3	A	1101	NDP	C3N-C2N-N1N	-2.16	120.01	123.10
3	F	1601	NDP	C3N-C2N-N1N	-2.16	120.01	123.10
3	E	1501	NDP	C3N-C2N-N1N	-2.08	120.13	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	NDP	C4A-C5A-N7A	-2.05	107.26	109.40

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1301	NDP	C5B-O5B-PA-O2A
3	C	1301	NDP	C3B-C2B-O2B-P2B
3	A	1101	NDP	C5B-O5B-PA-O1A
3	A	1101	NDP	C5B-O5B-PA-O2A
3	A	1101	NDP	C3B-C2B-O2B-P2B
3	A	1101	NDP	C5D-O5D-PN-O1N
3	D	1401	NDP	C5B-O5B-PA-O1A
3	D	1401	NDP	C5B-O5B-PA-O2A
3	D	1401	NDP	C3B-C2B-O2B-P2B
3	D	1401	NDP	C5D-O5D-PN-O1N
3	F	1601	NDP	C5B-O5B-PA-O1A
3	F	1601	NDP	C5B-O5B-PA-O2A
3	F	1601	NDP	C3B-C2B-O2B-P2B
3	F	1601	NDP	C5D-O5D-PN-O1N
3	E	1501	NDP	C5B-O5B-PA-O2A
3	E	1501	NDP	C3B-C2B-O2B-P2B
3	B	1201	NDP	C5B-O5B-PA-O1A
3	B	1201	NDP	C5B-O5B-PA-O2A
3	B	1201	NDP	C3B-C2B-O2B-P2B
3	B	1201	NDP	C5D-O5D-PN-O1N
3	A	1101	NDP	C2D-C1D-N1N-C2N
3	E	1501	NDP	C2D-C1D-N1N-C2N
4	A	1102	AKG	C1-C2-C3-C4
4	D	1402	AKG	C1-C2-C3-C4
4	C	1302	AKG	C1-C2-C3-C4
3	F	1601	NDP	PN-O3-PA-O1A
3	C	1301	NDP	C2D-C1D-N1N-C2N
3	B	1201	NDP	C2D-C1D-N1N-C2N
4	A	1102	AKG	O5-C2-C3-C4
4	C	1302	AKG	O5-C2-C3-C4
4	D	1402	AKG	O5-C2-C3-C4
3	A	1101	NDP	C2D-C1D-N1N-C6N
3	F	1601	NDP	C2D-C1D-N1N-C2N
3	A	1101	NDP	C2B-O2B-P2B-O1X
3	D	1401	NDP	C2B-O2B-P2B-O1X
3	E	1501	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	D	1401	NDP	C2D-C1D-N1N-C2N
3	E	1501	NDP	C2D-C1D-N1N-C6N
3	C	1301	NDP	C5B-O5B-PA-O3
3	A	1101	NDP	C5D-O5D-PN-O3
3	D	1401	NDP	C5D-O5D-PN-O3
3	F	1601	NDP	C5D-O5D-PN-O3
3	E	1501	NDP	C5B-O5B-PA-O3
3	B	1201	NDP	C2B-O2B-P2B-O2X
3	B	1201	NDP	C5D-O5D-PN-O3
3	C	1301	NDP	O4D-C1D-N1N-C2N
3	A	1101	NDP	O4D-C1D-N1N-C2N
3	E	1501	NDP	O4D-C1D-N1N-C2N
3	B	1201	NDP	O4D-C1D-N1N-C2N
3	B	1201	NDP	C2D-C1D-N1N-C6N
3	C	1301	NDP	C5B-O5B-PA-O1A
3	C	1301	NDP	C5D-O5D-PN-O2N
3	A	1101	NDP	C5D-O5D-PN-O2N
3	D	1401	NDP	C5D-O5D-PN-O2N
3	F	1601	NDP	C5D-O5D-PN-O2N
3	E	1501	NDP	C5B-O5B-PA-O1A
3	E	1501	NDP	C5D-O5D-PN-O2N
3	B	1201	NDP	C5D-O5D-PN-O2N
3	D	1401	NDP	O4D-C1D-N1N-C2N
3	C	1301	NDP	C2D-C1D-N1N-C6N
3	F	1601	NDP	O4D-C1D-N1N-C2N
4	B	1202	AKG	O5-C2-C3-C4
4	B	1202	AKG	C1-C2-C3-C4
3	D	1401	NDP	C2D-C1D-N1N-C6N
3	F	1601	NDP	C2D-C1D-N1N-C6N
3	A	1101	NDP	O4D-C1D-N1N-C6N
3	E	1501	NDP	O4D-C1D-N1N-C6N
3	B	1201	NDP	O4D-C1D-N1N-C6N
3	C	1301	NDP	O4D-C1D-N1N-C6N
3	C	1301	NDP	C2B-O2B-P2B-O1X
3	F	1601	NDP	C2B-O2B-P2B-O1X
3	D	1401	NDP	O4D-C1D-N1N-C6N
3	F	1601	NDP	O4D-C1D-N1N-C6N
3	C	1301	NDP	C2B-O2B-P2B-O2X
3	A	1101	NDP	C5B-O5B-PA-O3
3	A	1101	NDP	C2B-O2B-P2B-O3X
3	D	1401	NDP	C5B-O5B-PA-O3
3	F	1601	NDP	C5B-O5B-PA-O3

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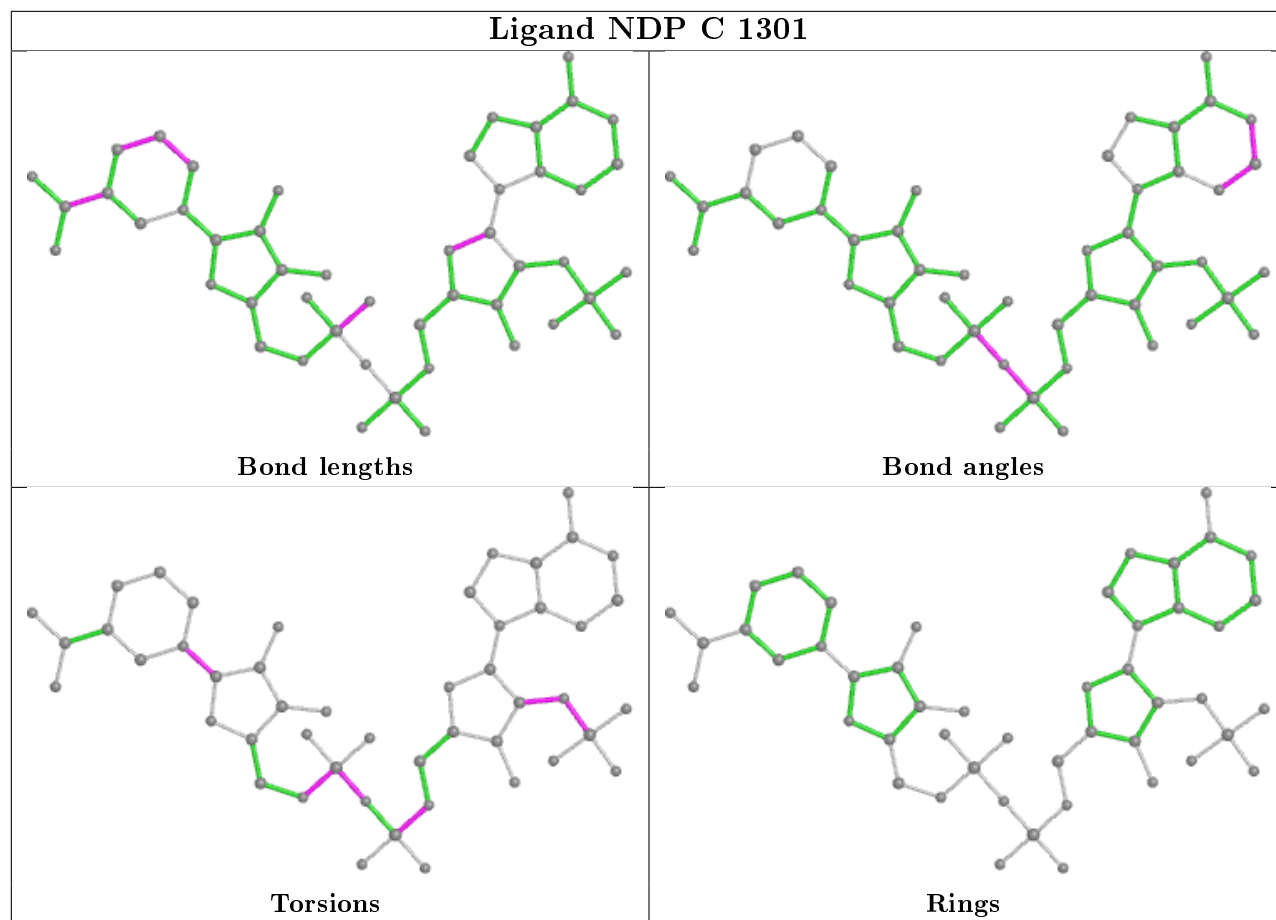
Mol	Chain	Res	Type	Atoms
3	B	1201	NDP	C5B-O5B-PA-O3
3	C	1301	NDP	PA-O3-PN-O2N
4	E	1502	AKG	C1-C2-C3-C4

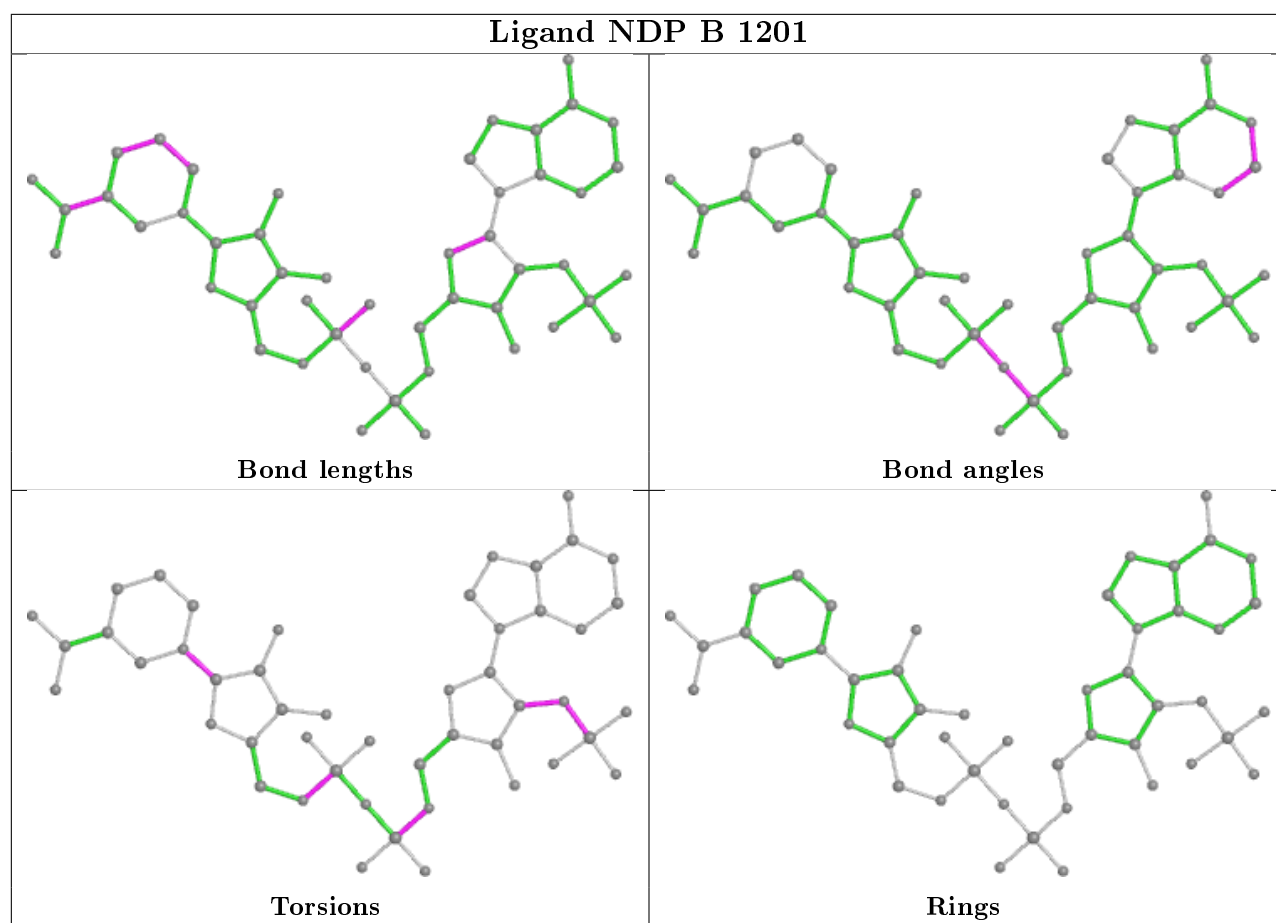
There are no ring outliers.

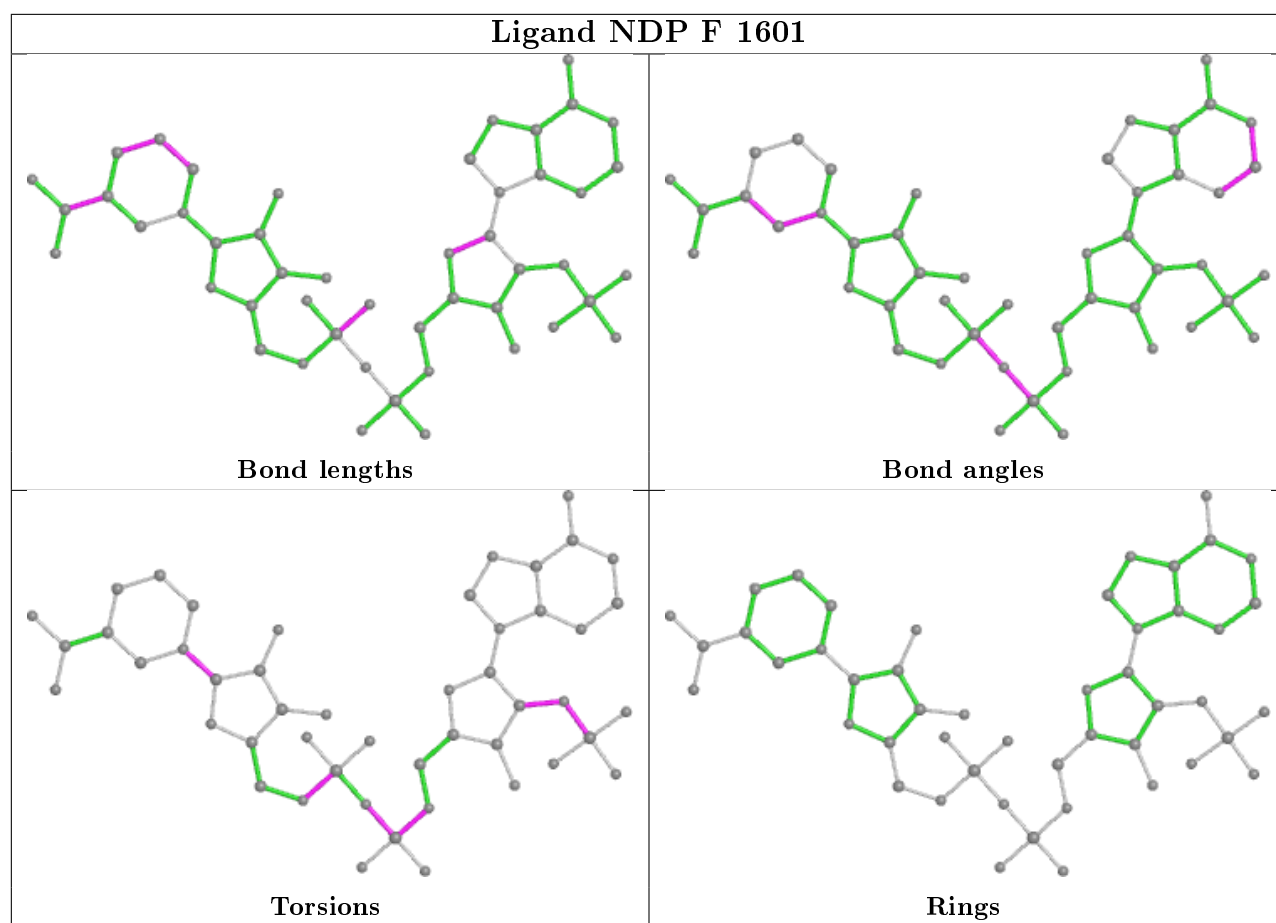
12 monomers are involved in 74 short contacts:

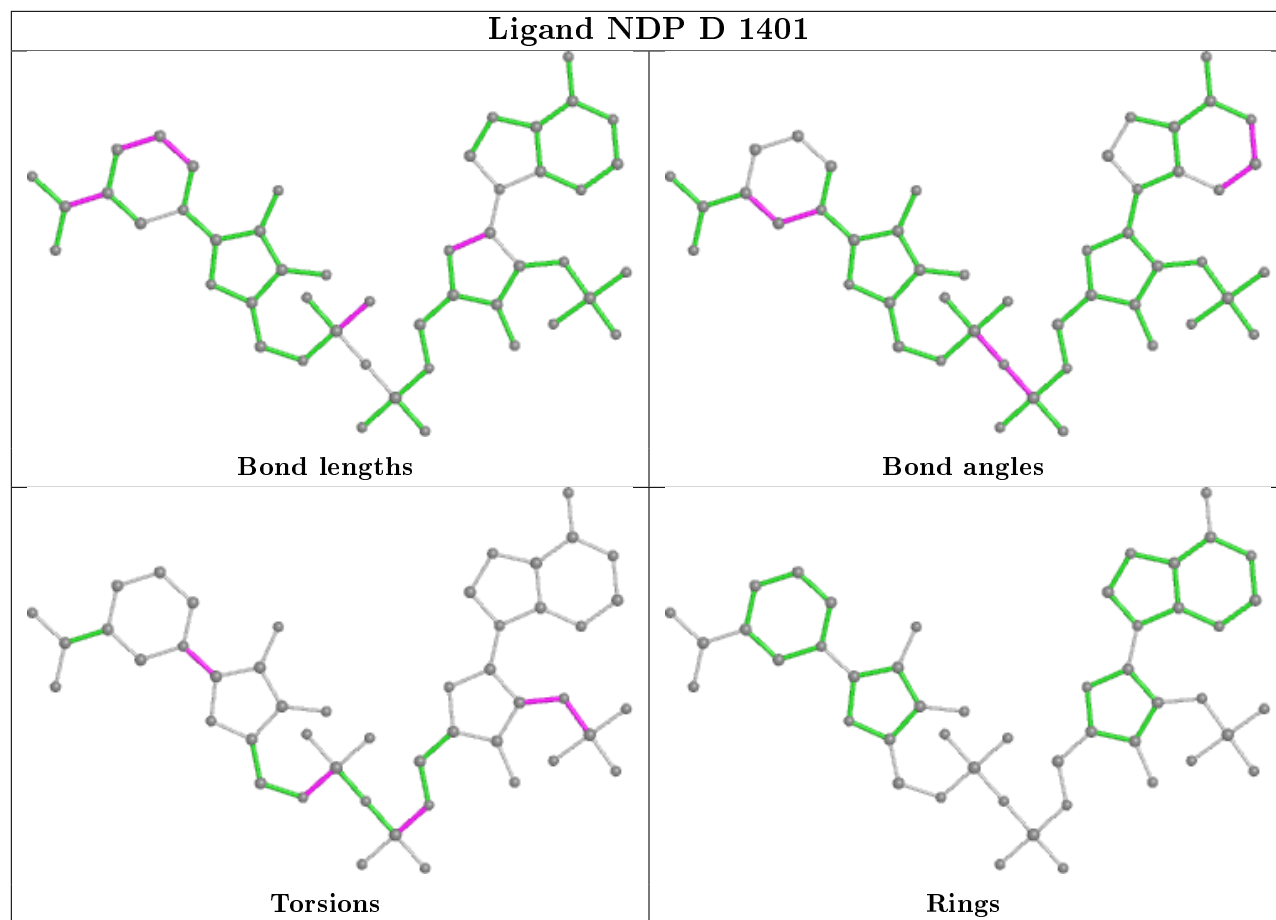
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	NDP	12	0
3	B	1201	NDP	13	0
4	E	1502	AKG	6	0
4	D	1402	AKG	5	0
4	B	1202	AKG	6	0
4	A	1102	AKG	7	0
3	F	1601	NDP	11	0
3	D	1401	NDP	12	0
4	C	1302	AKG	6	0
3	E	1501	NDP	12	0
3	A	1101	NDP	13	0
4	F	1602	AKG	5	0

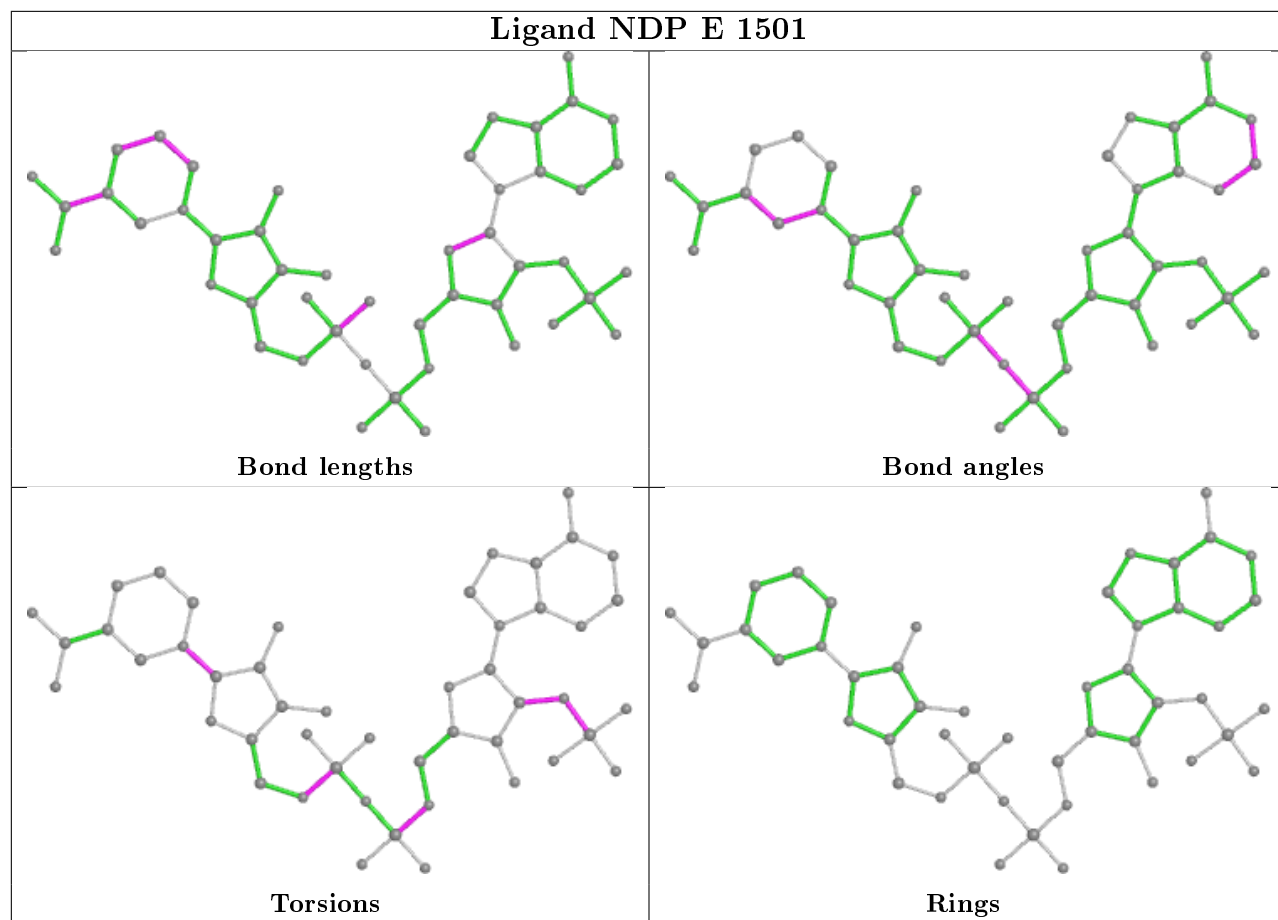
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

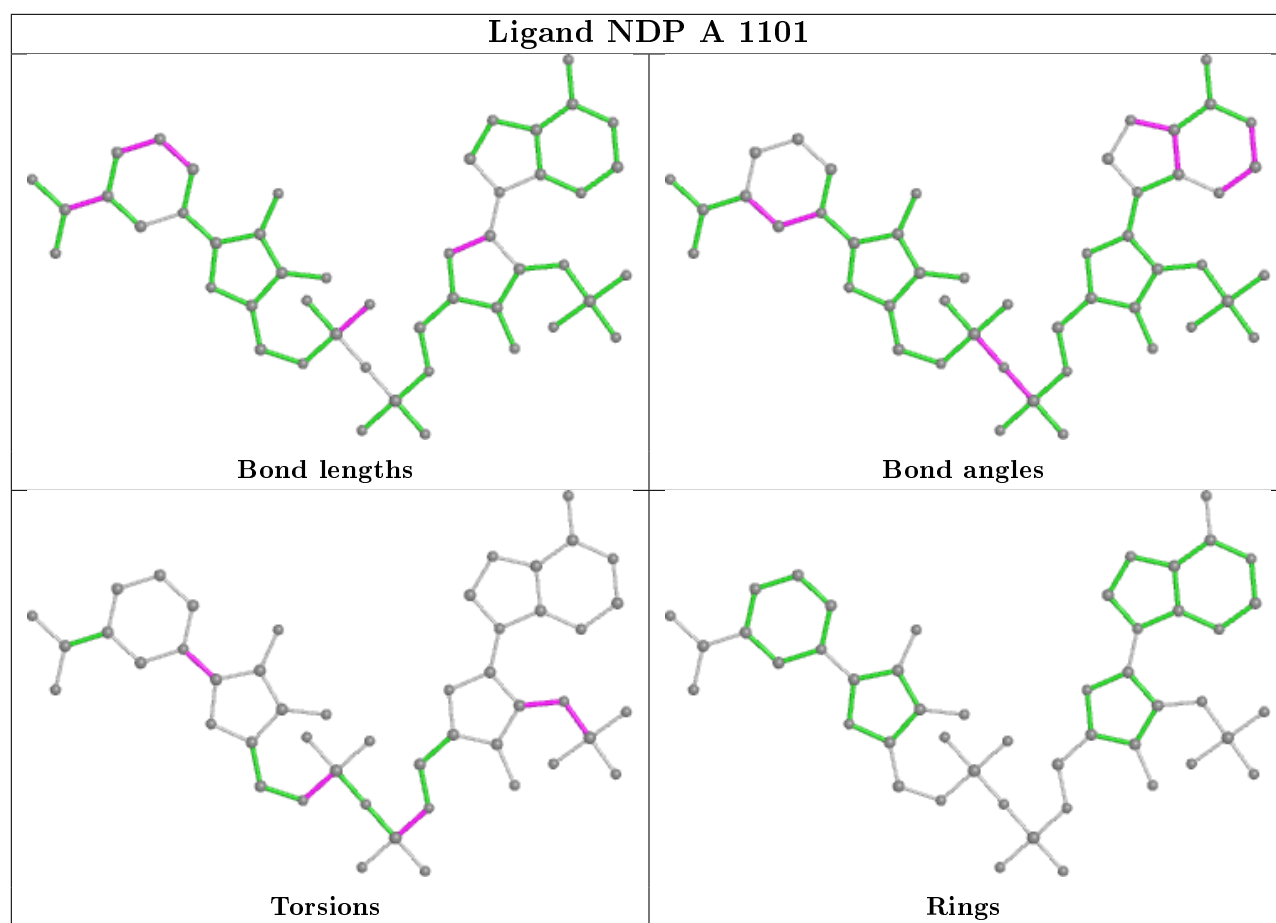












5.7 Other polymers [i](#)

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	410/427 (96%)	0.16	11 (2%) 54 55	42, 70, 111, 142	0
1	B	410/427 (96%)	0.23	17 (4%) 37 36	44, 66, 102, 148	0
1	C	410/427 (96%)	0.18	18 (4%) 34 33	36, 63, 97, 152	0
1	D	410/427 (96%)	0.25	17 (4%) 37 36	40, 63, 99, 135	0
1	E	410/427 (96%)	0.16	10 (2%) 59 60	45, 67, 104, 156	0
1	F	410/427 (96%)	0.18	12 (2%) 51 52	40, 61, 96, 141	0
All	All	2460/2562 (96%)	0.19	85 (3%) 44 44	36, 66, 103, 156	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	PHE	7.3
1	F	2	PHE	7.2
1	D	160	SER	5.8
1	C	164	THR	4.5
1	F	164	THR	4.5
1	D	2	PHE	4.4
1	A	2	PHE	4.4
1	C	2	PHE	4.4
1	B	2	PHE	4.1
1	D	156	VAL	4.1
1	D	165	ALA	4.0
1	C	165	ALA	3.8
1	D	153	LEU	3.8
1	C	148	PRO	3.7
1	C	153	LEU	3.7
1	B	148	PRO	3.5
1	C	163	THR	3.5
1	B	390	ALA	3.5
1	F	155	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	164	THR	3.4
1	E	167	PRO	3.4
1	B	153	LEU	3.4
1	B	374	ILE	3.4
1	E	157	TYR	3.3
1	D	148	PRO	3.2
1	C	410	LYS	3.2
1	D	162	PRO	3.2
1	A	241	PHE	3.0
1	B	411	SER	3.0
1	C	155	LEU	3.0
1	D	157	TYR	3.0
1	A	155	LEU	3.0
1	B	326	GLU	2.9
1	D	155	LEU	2.9
1	C	156	VAL	2.9
1	D	278	VAL	2.9
1	A	167	PRO	2.8
1	C	280	SER	2.8
1	B	155	LEU	2.8
1	F	150	PRO	2.7
1	C	147	ILE	2.7
1	B	278	VAL	2.7
1	C	117	ARG	2.7
1	D	282	ILE	2.6
1	D	166	GLN	2.6
1	E	155	LEU	2.5
1	C	387	GLU	2.5
1	E	274	TYR	2.5
1	D	244	LEU	2.5
1	B	386	ASN	2.4
1	A	235	ALA	2.4
1	A	237	TYR	2.4
1	B	203	ILE	2.4
1	E	161	ASP	2.3
1	A	206	LYS	2.3
1	D	158	LYS	2.3
1	D	159	PRO	2.3
1	B	281	ASP	2.3
1	F	161	ASP	2.3
1	A	164	THR	2.2
1	B	407	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	164	THR	2.2
1	F	411	SER	2.2
1	E	169	THR	2.2
1	F	407	LYS	2.2
1	F	247	HIS	2.2
1	D	91	LYS	2.2
1	F	207	LEU	2.2
1	B	356	LYS	2.2
1	C	162	PRO	2.2
1	C	278	VAL	2.1
1	B	275	ASP	2.1
1	C	276	GLY	2.1
1	C	407	LYS	2.1
1	C	6	LYS	2.1
1	D	374	ILE	2.1
1	F	169	THR	2.1
1	F	167	PRO	2.0
1	A	160	SER	2.0
1	A	274	TYR	2.0
1	A	386	ASN	2.0
1	E	411	SER	2.0
1	F	275	ASP	2.0
1	B	176	LYS	2.0
1	E	150	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

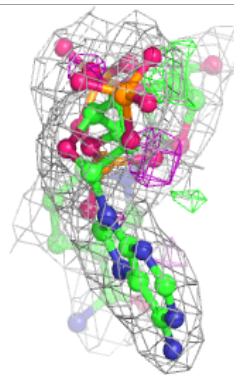
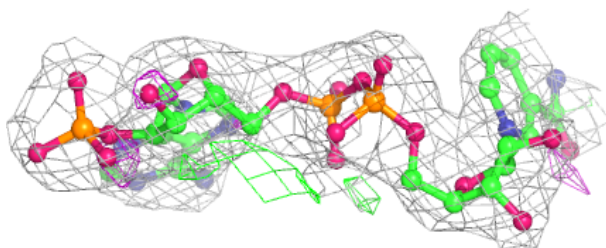
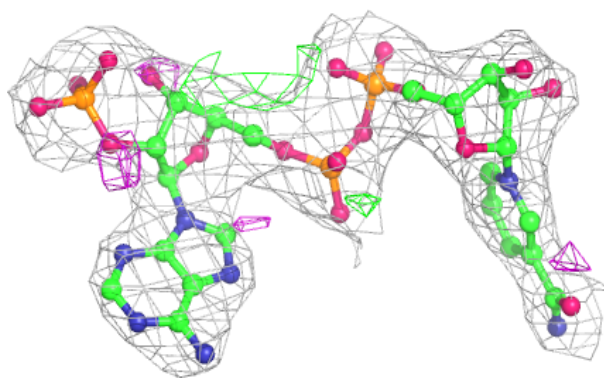
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	AKG	E	1502	10/10	0.89	0.34	69,77,80,80	0
4	AKG	A	1102	10/10	0.90	0.34	76,82,84,86	0
4	AKG	C	1302	10/10	0.91	0.33	65,69,72,72	0
4	AKG	F	1602	10/10	0.91	0.36	59,65,67,69	0
4	AKG	D	1402	10/10	0.93	0.23	51,64,67,69	0
4	AKG	B	1202	10/10	0.93	0.37	62,67,71,72	0
2	CA	D	1403	1/1	0.93	0.35	65,65,65,65	0
2	CA	B	1203	1/1	0.94	0.39	68,68,68,68	0
3	NDP	B	1201	48/48	0.94	0.19	53,61,70,75	0
2	CA	A	1103	1/1	0.94	0.33	64,64,64,64	0
3	NDP	F	1601	48/48	0.94	0.21	39,55,61,65	0
3	NDP	E	1501	48/48	0.95	0.18	42,59,66,69	0
3	NDP	A	1101	48/48	0.95	0.18	39,50,55,59	0
3	NDP	C	1301	48/48	0.96	0.19	38,44,48,55	0
3	NDP	D	1401	48/48	0.96	0.19	48,54,61,67	0
2	CA	E	1503	1/1	0.96	0.31	60,60,60,60	0
2	CA	F	1603	1/1	0.98	0.39	65,65,65,65	0
2	CA	C	1303	1/1	0.98	0.28	54,54,54,54	0

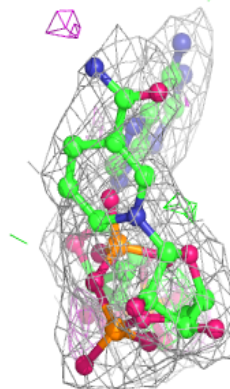
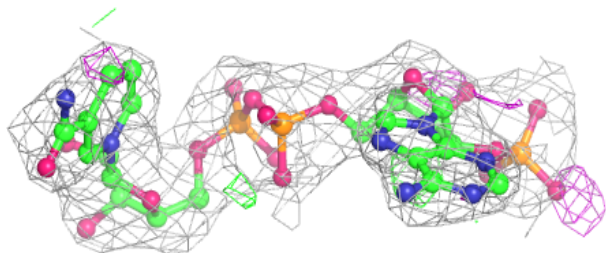
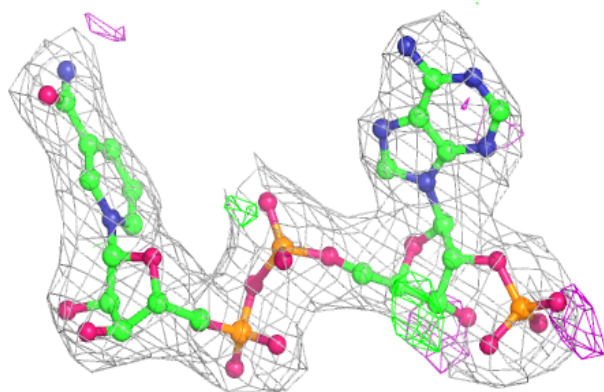
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NDP B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

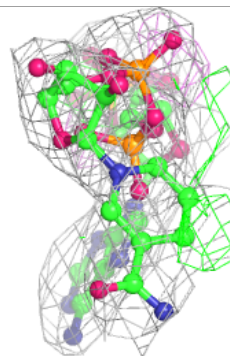
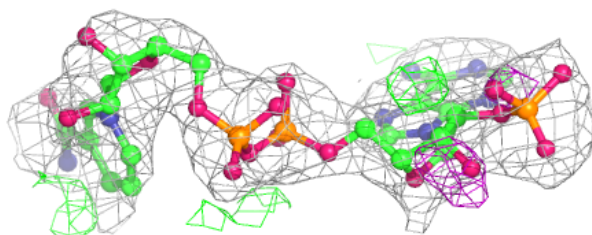
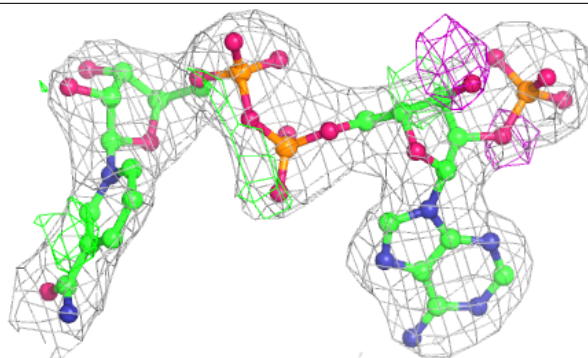
**Electron density around NDP F 1601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

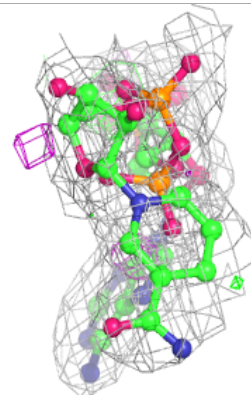
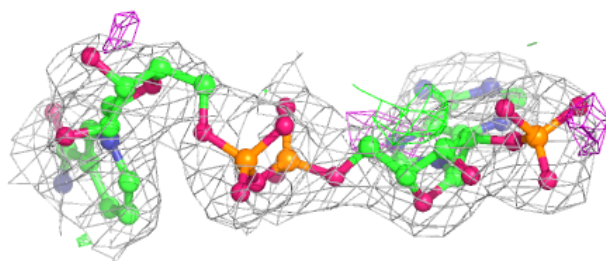
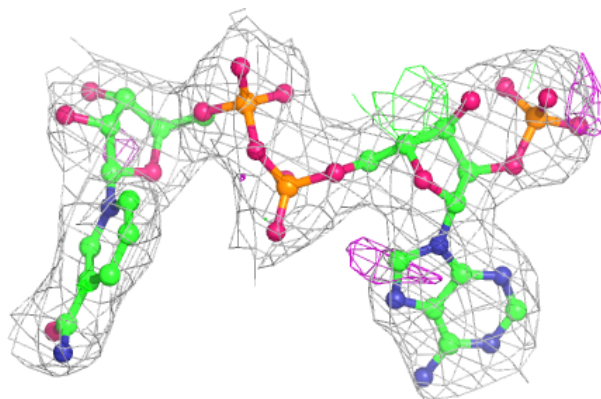


Electron density around NDP E 1501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

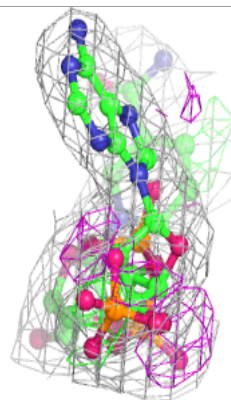
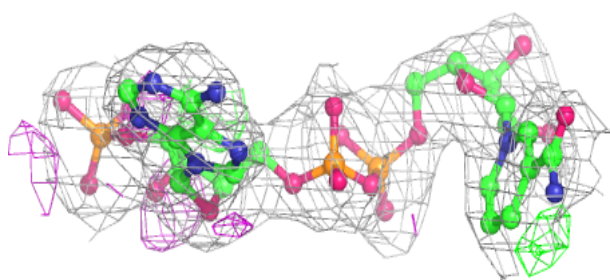
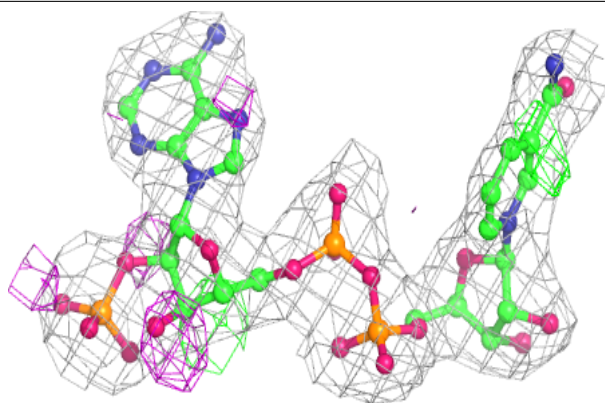
**Electron density around NDP A 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

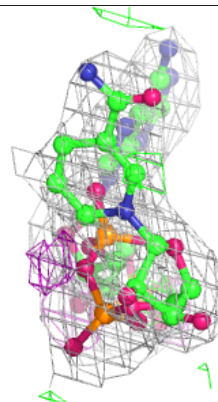
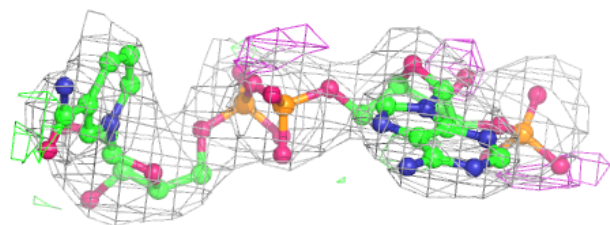
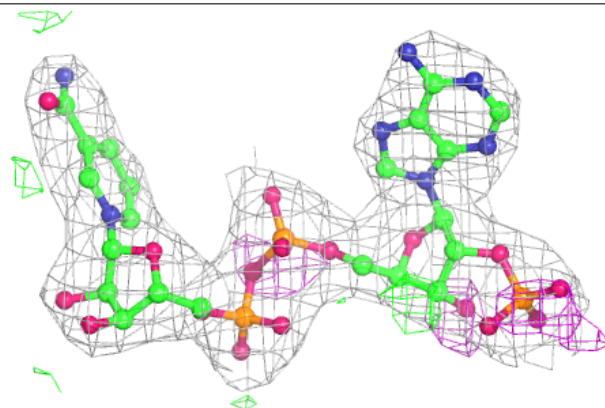


Electron density around NDP C 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NDP D 1401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.