Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2021 – 01:11 PM BST

PDB ID	:	7NOT
Title	:	Crystal structure of Mycobacterium tuberculosis ArgC in complex with nicotinamide adenine dinucleotide phosphate (NADP+) and 5-Methoxy-3-indoleacetic acid
Authors	:	Gupta, P.; Mendes, V.; Blundell, T.L.
Deposited on	:	2021-02-25
Resolution	:	2.54 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:

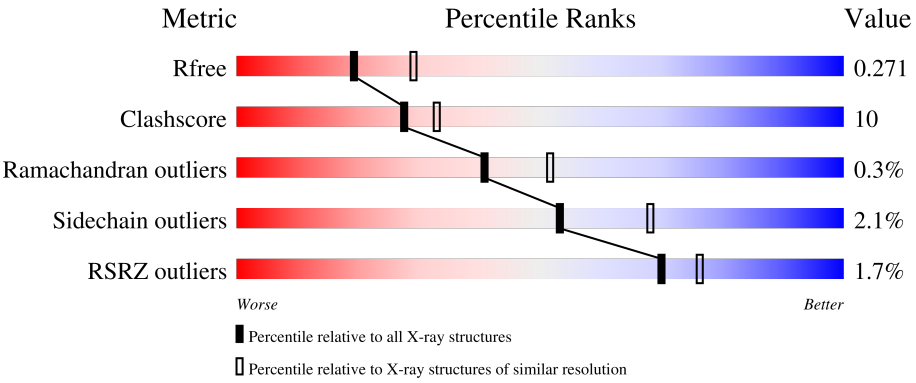
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	344	2% 75% 24%
1	B	344	2% 77% 23%
1	C	344	% 74% 26%
1	D	344	% 80% 20%
1	E	344	3% 81% 18%

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Mol	Chain	Length	Quality of chain
1	F	344	83% 16%
1	G	344	% 79% 20%
1	H	344	3% 74% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYI	A	401	-	-	X	-

2 Entry composition

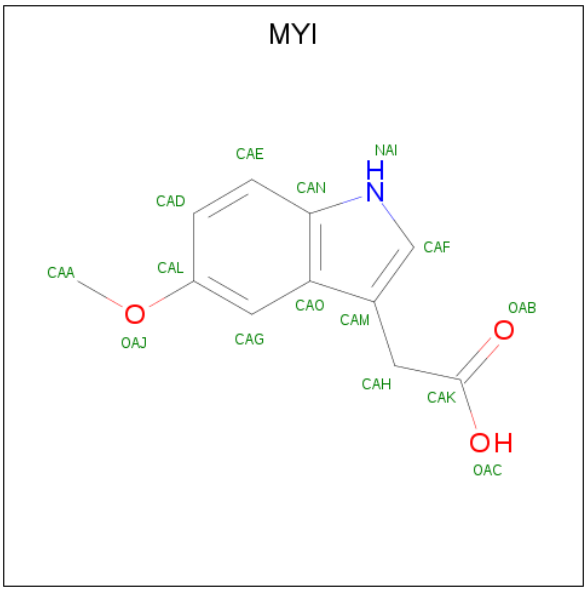
There are 4 unique types of molecules in this entry. The entry contains 20100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-acetyl-gamma-glutamyl-phosphate reductase.

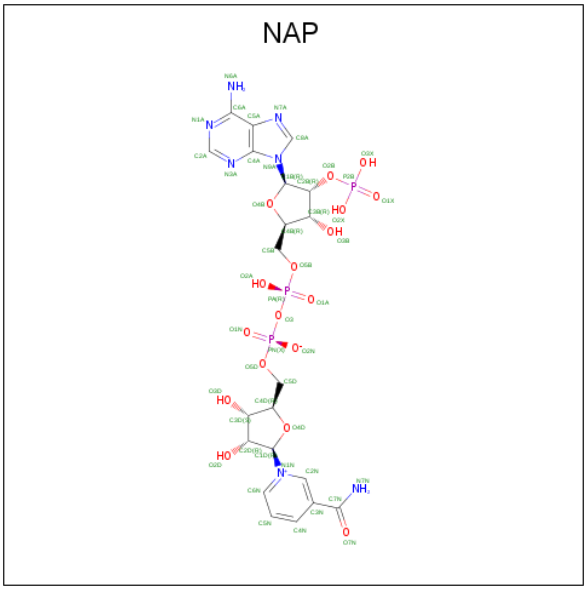
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2484	1570	446	463	5			
1	B	344	Total	C	N	O	S	0	0	0
			2469	1560	444	460	5			
1	C	344	Total	C	N	O	S	0	0	0
			2483	1568	444	466	5			
1	D	344	Total	C	N	O	S	0	0	0
			2491	1574	448	464	5			
1	E	344	Total	C	N	O	S	0	0	0
			2473	1563	440	465	5			
1	F	344	Total	C	N	O	S	0	0	0
			2474	1565	439	465	5			
1	G	344	Total	C	N	O	S	0	0	0
			2481	1569	442	465	5			
1	H	344	Total	C	N	O	S	0	0	0
			2451	1550	437	459	5			

- Molecule 2 is (5-methoxy-1H-indol-3-yl)acetic acid (three-letter code: MYI) (formula: $C_{11}H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	1	3		
2	B	1	Total	C	N	O	0	0
			15	11	1	3		
2	C	1	Total	C	N	O	0	0
			15	11	1	3		
2	D	1	Total	C	N	O	0	0
			15	11	1	3		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

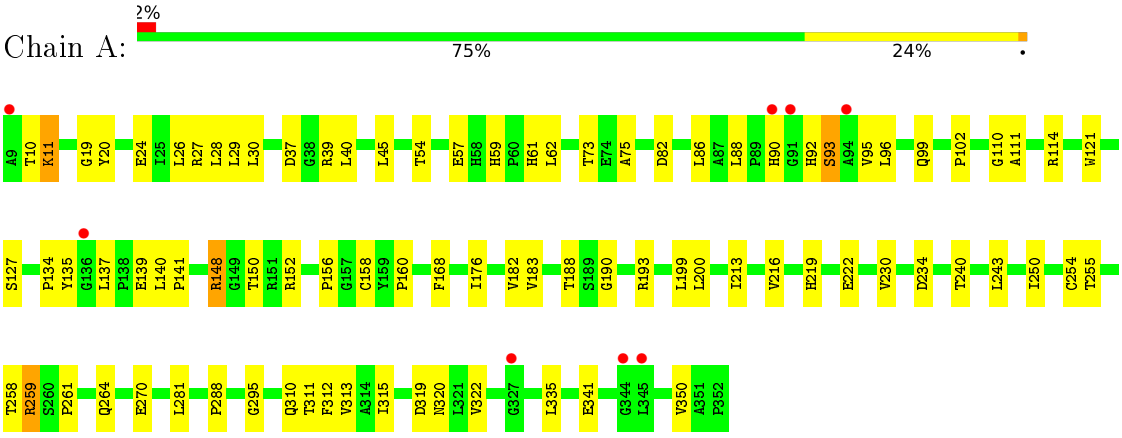
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	13	Total	O	0	0
			13	13		
4	C	15	Total	O	0	0
			15	15		
4	D	23	Total	O	0	0
			23	23		
4	E	16	Total	O	0	0
			16	16		
4	F	22	Total	O	0	0
			22	22		
4	G	24	Total	O	0	0
			24	24		
4	H	13	Total	O	0	0
			13	13		

3 Residue-property plots (i)

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.

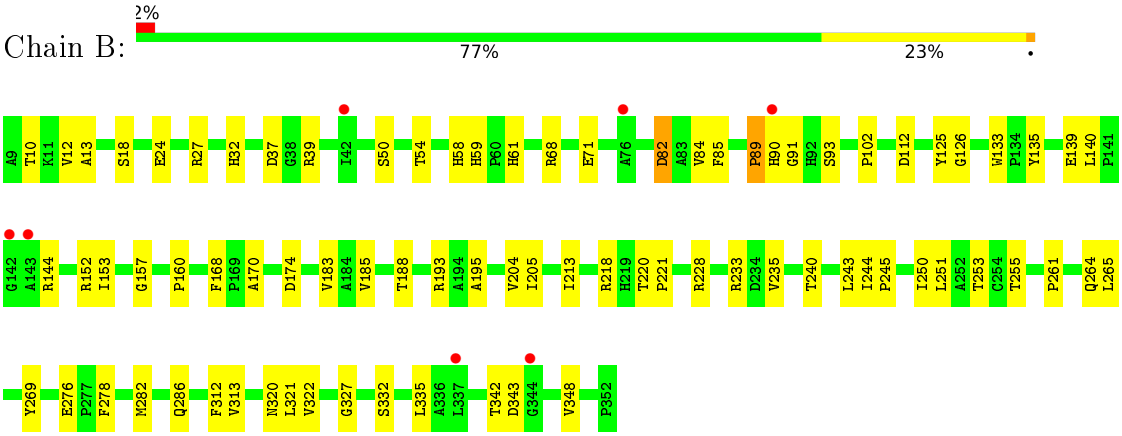
- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

Chain A:



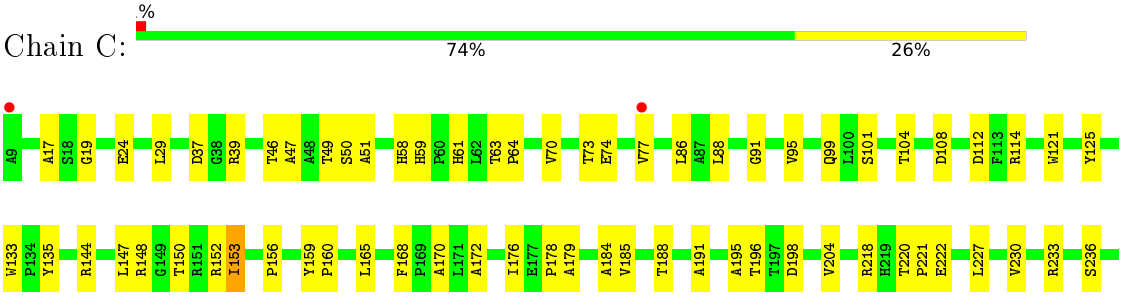
- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

Chain B:

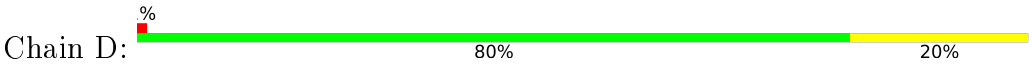


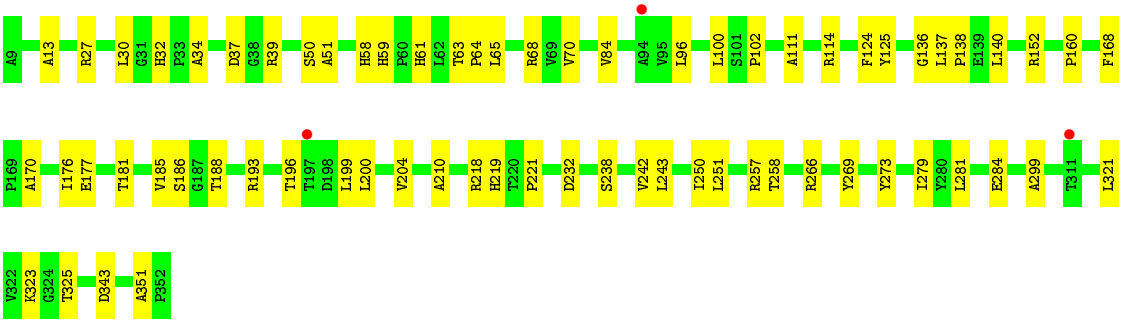
- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase

Chain C:

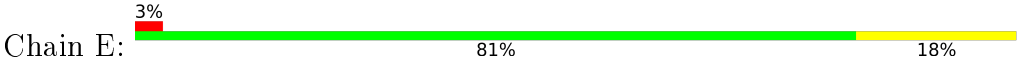


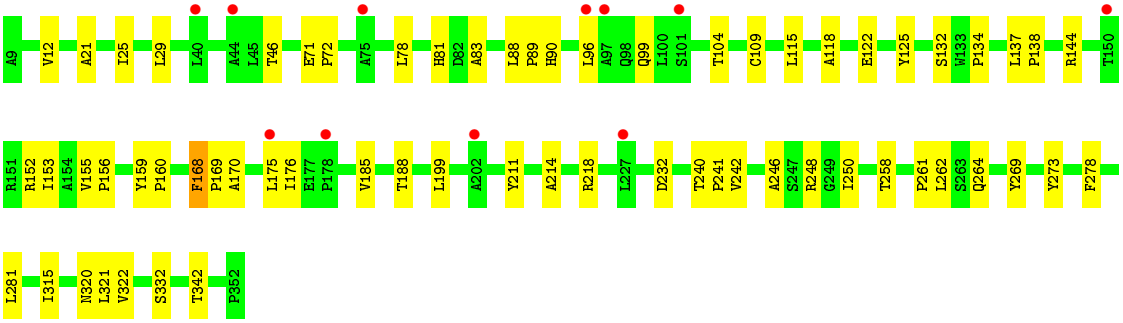
• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase



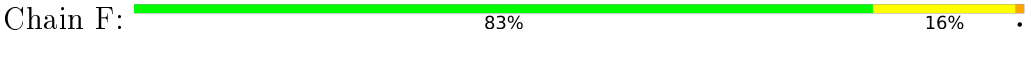


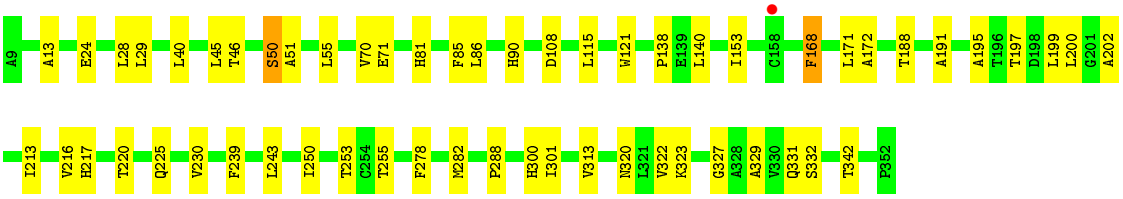
• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase



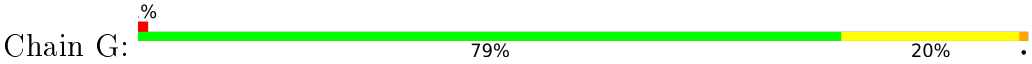


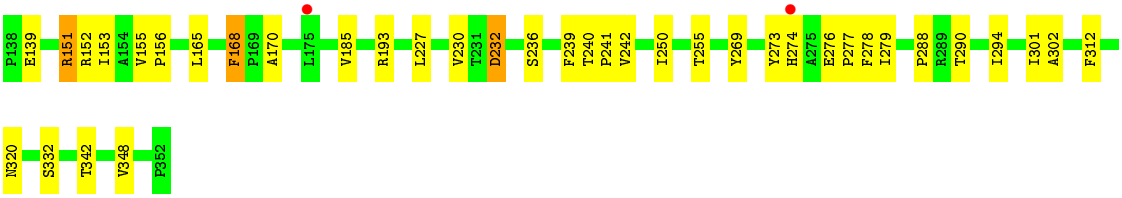
• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase



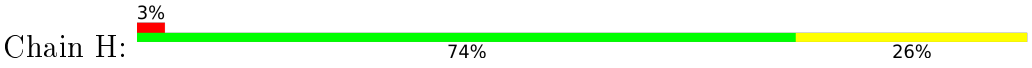


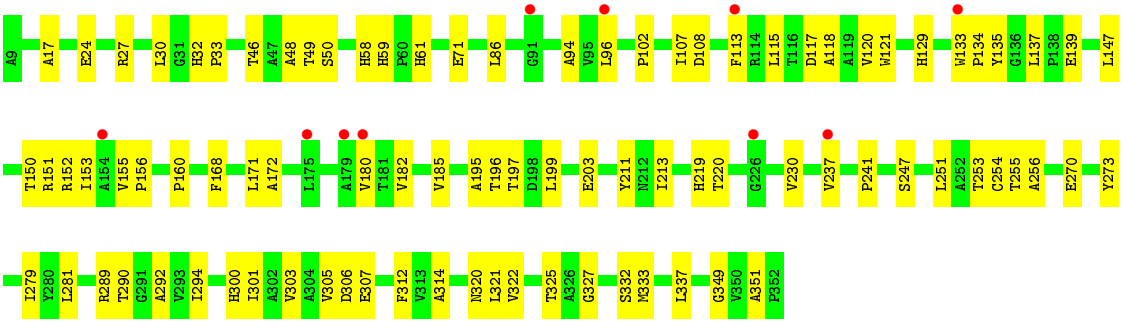
• Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase





- Molecule 1: N-acetyl-gamma-glutamyl-phosphate reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.40Å 132.00Å 124.55Å 90.00° 97.06° 90.00°	Depositor
Resolution (Å)	58.44 – 2.54 63.91 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.44-2.54) 99.3 (63.91-2.54)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.202 , 0.278 0.211 , 0.271	Depositor DCC
R_{free} test set	4348 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20100	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAP, MYI

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	0.54	0/2539	0.72	0/3477
1	B	0.51	0/2524	0.65	0/3459
1	C	0.57	0/2539	0.67	0/3478
1	D	0.48	0/2547	0.66	0/3487
1	E	0.58	0/2529	0.70	0/3467
1	F	0.52	0/2530	0.70	0/3468
1	G	0.53	0/2537	0.66	0/3476
1	H	0.52	0/2507	0.69	0/3440
All	All	0.53	0/20252	0.68	0/27752

There are no bond length outliers.

There are no bond angle outliers.

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	2484	0	2486	58	0
1	B	2469	0	2456	50	0
1	C	2483	0	2471	71	0
1	D	2491	0	2490	45	0
1	E	2473	0	2448	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2474	0	2460	36	0
1	G	2481	0	2473	46	0
1	H	2451	0	2404	66	0
2	A	15	0	10	7	0
2	B	15	0	10	2	0
2	C	15	0	10	5	0
2	D	15	0	10	1	0
3	C	48	0	24	3	0
3	D	48	0	24	3	0
4	A	12	0	0	0	0
4	B	13	0	0	0	0
4	C	15	0	0	2	0
4	D	23	0	0	1	0
4	E	16	0	0	1	0
4	F	22	0	0	1	0
4	G	24	0	0	0	0
4	H	13	0	0	0	0
All	All	20100	0	19776	397	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 10.

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:OE2	1:D:257:ARG:HD3	1.67	0.95
1:A:90:HIS:H	1:A:110:GLY:HA2	1.32	0.92
1:C:47:ALA:O	1:C:73:THR:HG23	1.72	0.89
1:C:147:LEU:HD22	1:C:153:ILE:HD13	1.59	0.85
1:H:290:THR:O	1:H:294:ILE:HG12	1.78	0.84
1:C:101:SER:OG	1:C:104:THR:HG23	1.78	0.84
1:B:91:GLY:HA2	1:B:112:ASP:OD2	1.80	0.80
1:E:12:VAL:HG22	1:E:83:ALA:HB3	1.63	0.80
1:E:248:ARG:NE	1:E:321:LEU:HD12	1.99	0.77
1:H:153:ILE:HD13	1:H:332:SER:HB3	1.65	0.76
1:B:243:LEU:HD13	2:B:401:MYI:HAE	1.67	0.76
1:A:188:THR:HG23	1:A:199:LEU:HD12	1.66	0.75
1:G:279:ILE:HD13	1:G:279:ILE:N	2.00	0.75
1:D:281:LEU:HD12	1:D:281:LEU:O	1.86	0.74
1:A:243:LEU:HD21	2:A:401:MYI:HAD	1.68	0.74
1:C:37:ASP:OD1	1:C:39:ARG:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:THR:HB	3:D:401:NAP:C5N	2.18	0.74
1:G:232:ASP:OD1	1:G:232:ASP:N	2.21	0.74
1:A:86:LEU:HD13	1:A:93:SER:HB2	1.70	0.73
1:A:19:GLY:HA2	1:A:193:ARG:HG3	1.72	0.72
1:C:153:ILE:HD12	1:C:332:SER:HB3	1.72	0.72
1:G:107:ILE:HG12	1:G:153:ILE:HD12	1.72	0.72
1:C:46:THR:OG1	1:C:73:THR:HG22	1.90	0.70
1:F:51:ALA:HA	1:F:70:VAL:O	1.91	0.70
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.56	0.70
1:B:139:GLU:OE1	1:B:139:GLU:N	2.24	0.70
1:G:51:ALA:HA	1:G:70:VAL:HG12	1.74	0.70
1:D:325:THR:HB	3:D:401:NAP:C4N	2.22	0.69
1:C:51:ALA:HA	1:C:70:VAL:HG12	1.74	0.69
1:D:13:ALA:HB3	1:D:84:VAL:HG22	1.74	0.69
1:H:139:GLU:OE2	1:H:139:GLU:N	2.23	0.68
1:A:102:PRO:HA	1:A:152:ARG:HH22	1.58	0.67
1:A:148:ARG:HG3	1:A:148:ARG:NH1	2.08	0.67
1:E:134:PRO:HD2	1:E:152:ARG:O	1.95	0.67
1:C:248:ARG:NH2	1:C:319:ASP:OD2	2.29	0.65
1:C:185:VAL:HG12	1:C:242:VAL:HB	1.77	0.65
1:D:51:ALA:HA	1:D:70:VAL:HG23	1.79	0.65
1:B:195:ALA:HA	1:D:200:LEU:HD21	1.79	0.65
1:D:176:ILE:HG22	1:D:258:THR:HB	1.79	0.65
1:H:180:VAL:CG2	1:H:237:VAL:HG22	2.27	0.64
1:A:20:TYR:CE1	1:A:193:ARG:HD3	2.33	0.64
1:C:250:ILE:HG13	1:C:320:ASN:HB3	1.80	0.63
1:C:325:THR:OG1	3:C:401:NAP:C4N	2.46	0.63
1:G:153:ILE:HD13	1:G:332:SER:HB3	1.80	0.63
1:C:101:SER:HG	1:C:104:THR:HG23	1.61	0.62
1:E:232:ASP:HA	4:E:402:HOH:O	1.98	0.62
1:F:188:THR:HG22	1:F:243:LEU:HD11	1.81	0.62
1:D:37:ASP:OD1	1:D:39:ARG:HG2	1.99	0.62
1:H:108:ASP:O	1:H:155:VAL:HG23	1.98	0.62
1:E:185:VAL:HG12	1:E:242:VAL:HB	1.82	0.62
1:A:288:PRO:HG2	1:A:315:ILE:HG22	1.82	0.62
1:C:188:THR:HG21	1:C:204:VAL:HG21	1.82	0.62
1:E:248:ARG:NE	1:E:321:LEU:CD1	2.63	0.62
1:D:266:ARG:NH2	1:D:284:GLU:HG3	2.15	0.61
1:H:185:VAL:HG22	1:H:251:LEU:HB3	1.82	0.61
1:D:181:THR:HG22	1:D:238:SER:HB3	1.83	0.61
1:E:248:ARG:HG2	1:E:321:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:THR:HG22	1:A:313:VAL:HG22	1.83	0.60
1:A:182:VAL:HG22	1:A:254:CYS:SG	2.42	0.60
1:A:10:THR:HA	1:A:82:ASP:OD2	2.02	0.60
1:D:196:THR:HB	1:D:199:LEU:HD12	1.82	0.60
1:C:86:LEU:HB2	1:C:108:ASP:HA	1.85	0.59
1:H:290:THR:O	1:H:294:ILE:CG1	2.50	0.59
1:C:46:THR:CB	1:C:73:THR:HG22	2.33	0.59
1:C:24:GLU:HG2	1:C:321:LEU:O	2.04	0.58
1:H:94:ALA:HA	1:H:113:PHE:HZ	1.68	0.58
1:H:102:PRO:HA	1:H:152:ARG:HH22	1.67	0.58
1:C:178:PRO:HG3	1:C:233:ARG:HD3	1.86	0.58
1:F:217:HIS:O	1:F:220:THR:HG23	2.02	0.58
1:B:12:VAL:HG11	1:B:85:PHE:HE1	1.68	0.58
1:C:133:TRP:CZ2	1:C:152:ARG:HD2	2.38	0.58
1:H:273:TYR:HB2	1:H:281:LEU:HD21	1.85	0.58
1:D:243:LEU:HD13	2:D:402:MYI:HAD	1.85	0.58
1:A:54:THR:OG1	1:A:57:GLU:HG3	2.04	0.58
1:C:74:GLU:HB2	1:C:77:VAL:HG23	1.86	0.58
1:B:188:THR:HG21	1:B:204:VAL:HG21	1.86	0.58
1:C:147:LEU:HD22	1:C:153:ILE:CD1	2.34	0.58
1:G:279:ILE:HG23	1:G:301:ILE:HD12	1.86	0.58
1:A:134:PRO:HD2	1:A:152:ARG:O	2.04	0.57
1:F:45:LEU:HD13	1:F:55:LEU:HD22	1.86	0.57
1:B:185:VAL:HG22	1:B:251:LEU:HB3	1.84	0.57
1:F:220:THR:HG22	1:F:239:PHE:HB3	1.87	0.57
1:D:30:LEU:HD11	1:D:65:LEU:HG	1.86	0.57
1:G:111:ALA:HA	1:G:114:ARG:HG3	1.86	0.57
1:A:183:VAL:HG22	1:A:240:THR:HB	1.86	0.57
1:A:350:VAL:HG22	1:B:27:ARG:NH1	2.19	0.57
1:B:322:VAL:O	1:B:327:GLY:N	2.38	0.56
1:F:86:LEU:HD12	1:F:108:ASP:HB2	1.88	0.56
1:G:102:PRO:HA	1:G:152:ARG:HH22	1.70	0.56
1:B:220:THR:N	1:B:221:PRO:HD2	2.21	0.56
1:E:273:TYR:HD2	1:E:281:LEU:HD21	1.71	0.56
1:B:82:ASP:OD1	1:B:82:ASP:N	2.37	0.56
1:E:88:LEU:HB3	1:E:89:PRO:CD	2.35	0.56
1:C:278:PHE:CZ	1:C:342:THR:HG22	2.41	0.55
1:E:278:PHE:CZ	1:E:342:THR:HG22	2.41	0.55
1:G:115:LEU:O	1:G:132:SER:HB3	2.06	0.55
1:H:172:ALA:HB2	1:H:230:VAL:HB	1.88	0.55
1:B:37:ASP:OD1	1:B:39:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ILE:HD12	1:E:332:SER:HB3	1.88	0.55
1:F:202:ALA:HA	1:H:247:SER:HB3	1.87	0.55
1:C:196:THR:HG22	1:C:198:ASP:H	1.72	0.55
1:G:108:ASP:O	1:G:155:VAL:HG23	2.06	0.55
1:H:86:LEU:HB2	1:H:108:ASP:OD1	2.07	0.55
1:C:185:VAL:HA	1:C:242:VAL:O	2.07	0.54
1:D:68:ARG:HD2	4:D:511:HOH:O	2.06	0.54
1:D:137:LEU:HD13	1:D:140:LEU:HG	1.88	0.54
1:E:137:LEU:HB2	1:E:156:PRO:HG2	1.89	0.54
1:A:259:ARG:HH11	1:A:310:GLN:NE2	2.05	0.54
1:A:261:PRO:HD2	1:A:264:GLN:OE1	2.08	0.54
1:B:144:ARG:NH2	1:B:276:GLU:OE1	2.37	0.54
1:H:50:SER:HB3	1:H:58:HIS:CE1	2.42	0.54
1:B:59:HIS:HB3	1:B:61:HIS:CE1	2.43	0.54
1:E:168:PHE:CD2	1:E:169:PRO:HD3	2.43	0.54
1:G:185:VAL:HG12	1:G:242:VAL:HB	1.88	0.54
1:H:117:ASP:HB3	1:H:120:VAL:HG12	1.89	0.54
1:A:135:TYR:CZ	1:A:156:PRO:HB3	2.43	0.54
1:B:174:ASP:OD1	1:B:233:ARG:NH1	2.41	0.54
1:C:172:ALA:HB2	1:C:230:VAL:HB	1.90	0.53
1:D:323:LYS:HD2	1:D:323:LYS:O	2.08	0.53
1:F:172:ALA:HB2	1:F:230:VAL:HB	1.89	0.53
1:F:300:HIS:C	1:F:301:ILE:HD13	2.28	0.53
1:E:175:LEU:O	1:E:258:THR:OG1	2.24	0.53
1:A:26:LEU:HD11	1:A:45:LEU:HD22	1.90	0.53
1:E:248:ARG:CD	1:E:321:LEU:HD12	2.38	0.53
1:C:147:LEU:O	1:C:150:THR:HG22	2.09	0.53
1:F:153:ILE:HD13	1:F:332:SER:HB3	1.90	0.53
1:B:102:PRO:HA	1:B:152:ARG:HH22	1.73	0.53
1:C:184:ALA:O	1:C:242:VAL:N	2.41	0.53
1:H:135:TYR:CZ	1:H:156:PRO:HB3	2.44	0.53
1:A:111:ALA:HA	1:A:114:ARG:HG3	1.91	0.52
1:A:121:TRP:NE1	1:A:127:SER:OG	2.41	0.52
1:H:322:VAL:O	1:H:327:GLY:N	2.41	0.52
1:A:190:GLY:HA3	2:A:401:MYI:CAF	2.39	0.52
1:H:32:HIS:CG	1:H:33:PRO:HD2	2.45	0.52
1:C:248:ARG:HG2	1:C:321:LEU:HD12	1.91	0.52
1:G:278:PHE:CZ	1:G:342:THR:HG22	2.44	0.52
1:H:320:ASN:O	1:H:325:THR:HG22	2.09	0.52
2:C:402:MYI:HAG	2:C:402:MYI:OAC	2.10	0.52
1:E:240:THR:HG21	1:H:253:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:MET:O	1:H:337:LEU:HG	2.09	0.52
1:A:140:LEU:HD22	1:A:141:PRO:HD2	1.91	0.52
1:A:139:GLU:OE1	1:A:139:GLU:N	2.40	0.51
1:A:243:LEU:HD21	2:A:401:MYI:CAD	2.39	0.51
1:A:90:HIS:N	1:A:110:GLY:HA2	2.14	0.51
1:F:195:ALA:HB2	1:H:197:THR:HG22	1.92	0.51
1:A:270:GLU:HG3	1:A:281:LEU:HD12	1.93	0.51
1:D:210:ALA:HB2	1:D:242:VAL:HG22	1.92	0.51
1:G:133:TRP:CD2	1:G:152:ARG:HB3	2.45	0.51
1:A:59:HIS:HB3	1:A:61:HIS:CE1	2.46	0.51
1:A:121:TRP:HE1	1:A:127:SER:HG	1.59	0.51
1:E:248:ARG:CG	1:E:321:LEU:HD12	2.42	0.51
1:H:134:PRO:HD2	1:H:152:ARG:O	2.11	0.51
1:G:139:GLU:OE1	1:G:139:GLU:N	2.43	0.50
1:H:17:ALA:O	1:H:59:HIS:HE1	1.94	0.50
1:A:295:GLY:N	1:A:319:ASP:OD2	2.34	0.50
1:C:191:ALA:HB2	2:C:402:MYI:CAD	2.42	0.50
1:H:312:PHE:CZ	1:H:314:ALA:HB2	2.46	0.50
1:B:250:ILE:HG13	1:B:320:ASN:HB3	1.94	0.50
1:C:165:LEU:HD13	1:C:279:ILE:HD12	1.93	0.50
1:H:279:ILE:HG23	1:H:301:ILE:HD12	1.93	0.50
1:H:107:ILE:HG12	1:H:153:ILE:HD12	1.93	0.50
1:D:96:LEU:O	1:D:100:LEU:HG	2.12	0.50
1:B:255:THR:HG22	1:B:313:VAL:HG22	1.94	0.49
1:H:59:HIS:HB3	1:H:61:HIS:CE1	2.48	0.49
1:H:24:GLU:HG2	1:H:321:LEU:HB3	1.93	0.49
1:B:213:ILE:HD13	1:C:315:ILE:CD1	2.43	0.49
1:D:102:PRO:HA	1:D:152:ARG:HH22	1.76	0.49
1:B:153:ILE:HD13	1:B:332:SER:HB3	1.93	0.49
1:D:321:LEU:HA	1:D:325:THR:HG22	1.94	0.49
1:G:17:ALA:O	1:G:59:HIS:NE2	2.42	0.49
1:C:73:THR:OG1	3:C:401:NAP:H2A	2.13	0.49
1:E:71:GLU:HB3	1:E:72:PRO:CD	2.43	0.49
1:E:138:PRO:HB2	1:E:144:ARG:NH2	2.27	0.49
1:H:290:THR:O	1:H:294:ILE:CD1	2.60	0.49
1:H:151:ARG:O	1:H:152:ARG:HD3	2.13	0.49
1:A:200:LEU:HD21	1:C:195:ALA:HA	1.94	0.49
1:D:58:HIS:O	1:D:193:ARG:NH2	2.44	0.49
1:F:191:ALA:HB3	1:F:199:LEU:HD21	1.95	0.49
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.77	0.48
1:B:133:TRP:CZ2	1:B:152:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLY:N	1:C:112:ASP:OD2	2.44	0.48
1:H:102:PRO:HA	1:H:152:ARG:NH2	2.27	0.48
1:E:109:CYS:HA	1:E:155:VAL:HB	1.95	0.48
1:E:188:THR:HG22	1:E:246:ALA:O	2.12	0.48
1:F:322:VAL:O	1:F:327:GLY:N	2.44	0.48
1:C:125:TYR:CE2	1:C:218:ARG:HD2	2.48	0.48
1:G:137:LEU:HB2	1:G:156:PRO:HG2	1.95	0.48
1:H:196:THR:OG1	1:H:199:LEU:HD12	2.14	0.48
1:H:303:VAL:HB	1:H:312:PHE:CE1	2.48	0.48
1:B:253:THR:HG21	1:C:240:THR:HG21	1.95	0.48
1:F:29:LEU:HD22	1:F:40:LEU:HD21	1.95	0.48
1:C:144:ARG:HG2	1:C:148:ARG:NH1	2.29	0.48
1:B:213:ILE:HD13	1:C:315:ILE:HD11	1.96	0.48
1:F:200:LEU:HD21	1:H:195:ALA:HA	1.95	0.48
1:C:220:THR:N	1:C:221:PRO:HD2	2.28	0.47
1:D:279:ILE:HD13	1:D:299:ALA:HB3	1.96	0.47
1:G:273:TYR:CG	1:G:279:ILE:HG21	2.48	0.47
1:D:125:TYR:CE2	1:D:218:ARG:HD3	2.49	0.47
1:A:75:ALA:HB2	1:A:99:GLN:HB2	1.97	0.47
1:B:133:TRP:CD2	1:B:152:ARG:HB3	2.49	0.47
1:D:170:ALA:HB2	1:D:269:TYR:HE1	1.79	0.47
1:G:255:THR:HA	1:G:312:PHE:O	2.15	0.47
1:C:114:ARG:HD3	1:C:222:GLU:OE2	2.15	0.47
1:F:213:ILE:O	1:F:216:VAL:HG22	2.14	0.47
1:H:220:THR:HG23	1:H:237:VAL:HG12	1.95	0.47
1:H:237:VAL:HG12	1:H:237:VAL:O	2.13	0.47
1:D:188:THR:HG22	1:D:243:LEU:HD11	1.96	0.46
1:H:305:VAL:HG12	1:H:307:GLU:HG3	1.97	0.46
1:C:61:HIS:CD2	1:D:351:ALA:HB3	2.50	0.46
1:C:112:ASP:HA	1:C:121:TRP:CH2	2.50	0.46
1:E:25:ILE:O	1:E:29:LEU:HG	2.15	0.46
1:F:138:PRO:HG2	1:F:331:GLN:NE2	2.29	0.46
1:G:227:LEU:O	1:G:230:VAL:HG22	2.16	0.46
1:F:278:PHE:CZ	1:F:342:THR:HG22	2.50	0.46
1:E:248:ARG:HG2	1:E:321:LEU:CD1	2.44	0.46
1:G:101:SER:OG	1:G:103:GLU:HG2	2.15	0.46
1:A:29:LEU:HD22	1:A:40:LEU:HD21	1.98	0.46
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.66	0.46
1:E:118:ALA:O	1:E:122:GLU:HG3	2.14	0.46
2:A:401:MYI:HAG	2:A:401:MYI:CAK	2.45	0.46
1:F:197:THR:HA	1:F:200:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PRO:HD2	1:B:264:GLN:HG3	1.98	0.46
1:E:90:HIS:O	1:E:90:HIS:CD2	2.69	0.46
1:F:140:LEU:HD23	1:F:140:LEU:HA	1.77	0.46
1:A:86:LEU:CD1	1:A:93:SER:HB2	2.44	0.46
1:D:124:PHE:CE1	1:D:221:PRO:HG3	2.51	0.46
1:C:281:LEU:HD13	4:C:511:HOH:O	2.16	0.46
1:F:13:ALA:HB2	1:F:81:HIS:CD2	2.50	0.46
1:H:160:PRO:HD3	1:H:219:HIS:ND1	2.31	0.46
1:D:188:THR:HG21	1:D:204:VAL:HG11	1.98	0.45
1:H:321:LEU:HA	1:H:325:THR:CG2	2.45	0.45
1:A:37:ASP:OD1	1:A:39:ARG:HG3	2.16	0.45
1:G:165:LEU:HD23	1:G:168:PHE:HE2	1.80	0.45
1:G:16:GLY:N	1:G:46:THR:O	2.42	0.45
1:G:105:LEU:HG	1:G:105:LEU:O	2.16	0.45
1:C:133:TRP:CD2	1:C:152:ARG:HB3	2.51	0.45
1:C:170:ALA:HB1	1:C:176:ILE:HG12	1.98	0.45
1:C:248:ARG:CG	1:C:321:LEU:HD12	2.47	0.45
1:D:111:ALA:HA	1:D:114:ARG:HG3	1.97	0.45
1:E:81:HIS:O	1:E:104:THR:HG23	2.16	0.45
1:E:125:TYR:CE2	1:E:218:ARG:HD3	2.51	0.45
1:C:159:TYR:CE2	2:C:402:MYI:HAHA	2.52	0.45
1:D:273:TYR:CD2	1:D:279:ILE:HG21	2.51	0.45
1:F:220:THR:HG22	1:F:239:PHE:HD2	1.81	0.45
1:H:30:LEU:HD23	1:H:30:LEU:HA	1.79	0.45
1:A:11:LYS:HB2	1:A:11:LYS:HE3	1.58	0.45
1:B:125:TYR:CE2	1:B:218:ARG:HD3	2.52	0.45
1:F:323:LYS:HB2	4:F:409:HOH:O	2.16	0.45
1:A:335:LEU:HG	1:A:341:GLU:HG3	1.99	0.45
1:C:135:TYR:OH	1:C:156:PRO:HB3	2.17	0.45
1:F:278:PHE:CE2	1:F:342:THR:HG22	2.51	0.44
1:G:250:ILE:HG13	1:G:320:ASN:HB3	1.97	0.44
1:A:176:ILE:HG22	1:A:258:THR:HB	1.99	0.44
1:A:213:ILE:O	1:A:216:VAL:HG22	2.17	0.44
1:D:193:ARG:HB2	3:D:401:NAP:O2A	2.17	0.44
1:E:90:HIS:O	1:E:90:HIS:CG	2.69	0.44
1:E:315:ILE:HD12	1:H:213:ILE:HD13	2.00	0.44
1:G:26:LEU:HD11	1:G:45:LEU:HD22	1.99	0.44
1:A:259:ARG:NH1	1:A:310:GLN:NE2	2.66	0.44
1:D:185:VAL:HG22	1:D:251:LEU:HB3	1.97	0.44
1:A:311:THR:HG22	1:A:312:PHE:O	2.18	0.44
1:B:133:TRP:CG	1:B:152:ARG:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:TYR:HB2	1:E:160:PRO:HD3	1.98	0.44
1:E:315:ILE:CD1	1:H:213:ILE:HD13	2.48	0.44
1:G:61:HIS:CG	1:H:351:ALA:HB3	2.52	0.44
1:B:205:ILE:HA	1:B:245:PRO:HB3	1.99	0.44
1:D:186:SER:HB2	1:D:250:ILE:HG12	2.00	0.44
1:G:30:LEU:HD11	1:G:65:LEU:HG	1.99	0.44
1:H:24:GLU:HG2	1:H:321:LEU:O	2.18	0.44
1:H:255:THR:HA	1:H:312:PHE:O	2.18	0.44
1:B:32:HIS:CE1	1:B:343:ASP:HB3	2.53	0.44
1:C:19:GLY:HA3	3:C:401:NAP:O5B	2.18	0.44
1:F:250:ILE:HG13	1:F:320:ASN:HB3	1.99	0.44
1:G:273:TYR:CD2	1:G:279:ILE:HG21	2.53	0.44
1:H:86:LEU:HD12	1:H:108:ASP:HB2	1.99	0.44
1:B:243:LEU:HD22	2:B:401:MYI:HAD	1.99	0.44
1:C:61:HIS:CG	1:D:351:ALA:HB3	2.53	0.43
1:C:95:VAL:O	1:C:99:GLN:HG3	2.18	0.43
1:B:126:GLY:HA2	1:G:99:GLN:OE1	2.18	0.43
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.90	0.43
1:F:115:LEU:HA	1:F:225:GLN:HE22	1.83	0.43
1:G:86:LEU:HB2	1:G:108:ASP:HA	1.98	0.43
1:B:335:LEU:HD23	1:B:335:LEU:HA	1.86	0.43
1:C:159:TYR:HB2	1:C:160:PRO:HD3	2.00	0.43
1:H:289:ARG:HG3	1:H:292:ALA:H	1.84	0.43
1:A:24:GLU:CD	1:A:27:ARG:HE	2.21	0.43
1:A:188:THR:O	1:A:188:THR:HG22	2.17	0.43
1:C:288:PRO:HD3	1:C:302:ALA:HB2	2.01	0.43
1:C:307:GLU:OE1	1:C:307:GLU:HA	2.19	0.43
1:D:136:GLY:O	1:D:138:PRO:HD3	2.18	0.43
1:E:21:ALA:O	1:E:25:ILE:HG13	2.18	0.43
1:F:282:MET:HG2	1:F:301:ILE:O	2.19	0.43
1:G:290:THR:O	1:G:294:ILE:HG13	2.19	0.43
1:H:96:LEU:HD23	1:H:96:LEU:HA	1.82	0.43
1:H:133:TRP:CD2	1:H:152:ARG:HB3	2.54	0.43
1:B:18:SER:O	1:B:193:ARG:NH1	2.48	0.43
1:C:63:THR:N	1:C:64:PRO:CD	2.81	0.43
1:C:101:SER:OG	1:C:104:THR:CG2	2.59	0.43
1:G:12:VAL:HA	1:G:83:ALA:O	2.19	0.43
1:C:251:LEU:HD21	1:C:315:ILE:CG2	2.48	0.43
1:F:288:PRO:HB3	1:F:300:HIS:HB3	2.00	0.43
1:D:34:ALA:HB1	1:D:39:ARG:HG3	2.00	0.43
1:A:26:LEU:HA	1:A:26:LEU:HD23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ALA:HA	1:C:236:SER:HB3	2.02	0.42
1:A:62:LEU:HA	1:B:348:VAL:HG13	2.00	0.42
1:F:253:THR:HG21	1:G:240:THR:HG21	2.01	0.42
1:H:211:TYR:O	1:H:241:PRO:HG2	2.18	0.42
1:B:12:VAL:HG11	1:B:85:PHE:CE1	2.51	0.42
1:C:24:GLU:HG3	1:C:326:ALA:HB3	2.00	0.42
1:G:288:PRO:HD3	1:G:302:ALA:HB2	2.02	0.42
1:B:278:PHE:CZ	1:B:342:THR:HG22	2.54	0.42
1:C:276:GLU:OE1	1:C:277:PRO:HD2	2.20	0.42
1:D:50:SER:O	1:D:70:VAL:CG2	2.67	0.42
1:D:160:PRO:HD3	1:D:219:HIS:ND1	2.34	0.42
1:F:171:LEU:HD12	1:F:171:LEU:HA	1.83	0.42
1:H:182:VAL:HG22	1:H:254:CYS:SG	2.59	0.42
1:A:73:THR:HG22	1:A:96:LEU:HD11	2.01	0.42
1:A:158:CYS:SG	2:A:401:MYI:HAF	2.59	0.42
1:D:63:THR:OG1	1:D:64:PRO:HD3	2.19	0.42
1:G:71:GLU:HB3	1:G:72:PRO:CD	2.50	0.42
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.78	0.42
1:D:34:ALA:CB	1:D:39:ARG:HG3	2.49	0.42
1:E:88:LEU:HB3	1:E:89:PRO:HD2	2.01	0.42
1:F:24:GLU:O	1:F:28:LEU:HG	2.19	0.42
1:F:85:PHE:HE1	1:F:329:ALA:HB1	1.85	0.42
1:F:255:THR:HG22	1:F:313:VAL:HG22	2.02	0.42
1:G:109:CYS:HA	1:G:155:VAL:HB	2.02	0.42
1:B:10:THR:HG23	1:B:82:ASP:HB2	2.01	0.42
1:B:170:ALA:HB2	1:B:269:TYR:HE1	1.85	0.42
1:B:228:ARG:HG3	1:B:235:VAL:HG22	2.02	0.42
1:D:32:HIS:CE1	1:D:343:ASP:HB3	2.55	0.42
1:G:276:GLU:HA	1:G:277:PRO:HD2	1.83	0.42
2:A:401:MYI:CAK	2:A:401:MYI:CAG	2.98	0.41
1:B:265:LEU:HD13	1:B:312:PHE:CD1	2.55	0.41
1:A:92:HIS:ND1	1:A:92:HIS:C	2.73	0.41
1:A:261:PRO:HG2	1:A:264:GLN:HB2	2.02	0.41
1:E:262:LEU:HA	1:E:262:LEU:HD12	1.80	0.41
1:B:244:ILE:HG21	1:C:244:ILE:HG21	2.02	0.41
1:C:46:THR:HB	1:C:73:THR:HG22	2.00	0.41
1:C:49:THR:HG23	4:C:515:HOH:O	2.19	0.41
1:E:115:LEU:O	1:E:132:SER:HB3	2.20	0.41
1:H:24:GLU:HA	1:H:24:GLU:OE1	2.21	0.41
1:B:54:THR:HA	1:B:68:ARG:O	2.19	0.41
1:B:282:MET:HE2	1:B:286:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:HG22	1:D:27:ARG:NH1	2.36	0.41
1:G:54:THR:HA	1:G:68:ARG:O	2.20	0.41
1:G:239:PHE:CE2	1:G:241:PRO:HG3	2.56	0.41
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.91	0.41
1:E:152:ARG:HA	1:E:152:ARG:HD3	1.84	0.41
1:E:211:TYR:O	1:E:241:PRO:HG2	2.21	0.41
1:A:20:TYR:CZ	1:A:193:ARG:HD3	2.55	0.41
1:E:248:ARG:CZ	1:E:321:LEU:HD12	2.49	0.41
1:G:348:VAL:HG12	1:H:27:ARG:HG3	2.02	0.41
1:H:115:LEU:HD12	1:H:121:TRP:HE3	1.85	0.41
1:C:297:ASN:O	1:C:323:LYS:HD3	2.20	0.41
1:F:168:PHE:CD1	1:F:168:PHE:C	2.94	0.41
1:G:61:HIS:HD2	1:H:349:GLY:O	2.02	0.41
1:G:348:VAL:CG1	1:H:27:ARG:HG3	2.51	0.41
1:C:227:LEU:O	1:C:230:VAL:HG22	2.20	0.41
1:E:214:ALA:HA	1:H:306:ASP:HB2	2.02	0.41
1:E:261:PRO:HG2	1:E:264:GLN:HB2	2.03	0.41
1:G:151:ARG:HA	1:G:151:ARG:HD2	1.78	0.41
1:H:46:THR:HA	1:H:71:GLU:O	2.21	0.41
1:A:135:TYR:OH	1:A:222:GLU:OE2	2.29	0.41
1:B:188:THR:HG22	1:B:243:LEU:HD11	2.02	0.41
1:C:191:ALA:HB1	2:C:402:MYI:HAAB	2.02	0.41
1:D:232:ASP:OD1	1:D:232:ASP:N	2.43	0.41
1:H:118:ALA:HA	1:H:129:HIS:ND1	2.36	0.41
1:H:171:LEU:HD12	1:H:171:LEU:HA	1.91	0.41
1:B:50:SER:HB3	1:B:58:HIS:NE2	2.36	0.40
1:B:183:VAL:HA	1:B:240:THR:O	2.20	0.40
1:E:46:THR:HG21	1:E:78:LEU:HD21	2.03	0.40
1:E:250:ILE:HG13	1:E:320:ASN:HB3	2.03	0.40
1:E:199:LEU:HD23	1:E:199:LEU:HA	1.91	0.40
1:F:46:THR:HA	1:F:71:GLU:O	2.22	0.40
1:H:303:VAL:HB	1:H:312:PHE:HE1	1.85	0.40
1:A:95:VAL:O	1:A:99:GLN:HG3	2.21	0.40
1:C:17:ALA:O	1:C:59:HIS:NE2	2.54	0.40
1:C:50:SER:HB2	1:C:58:HIS:CE1	2.56	0.40
1:C:159:TYR:HE2	2:C:402:MYI:HAHA	1.86	0.40
1:F:115:LEU:HD12	1:F:121:TRP:HE3	1.85	0.40
1:H:107:ILE:CD1	1:H:333:MET:HB2	2.51	0.40
1:B:13:ALA:HB3	1:B:84:VAL:HG22	2.02	0.40
1:B:24:GLU:HG2	1:B:321:LEU:HB3	2.03	0.40
1:B:157:GLY:C	1:B:160:PRO:HD2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:GLU:HB3	1:C:279:ILE:HG12	2.02	0.40
1:D:59:HIS:HB3	1:D:61:HIS:CE1	2.57	0.40
1:E:170:ALA:HB2	1:E:269:TYR:CE1	2.57	0.40
1:E:185:VAL:HA	1:E:242:VAL:O	2.22	0.40
1:G:170:ALA:HB2	1:G:269:TYR:HE1	1.87	0.40
1:H:147:LEU:O	1:H:150:THR:HG22	2.22	0.40
1:A:160:PRO:HD3	1:A:219:HIS:ND1	2.36	0.40
2:A:401:MYI:CAG	2:A:401:MYI:OAC	2.70	0.40
1:E:176:ILE:HG22	1:E:258:THR:HB	2.03	0.40
1:G:61:HIS:HB3	1:H:292:ALA:HA	2.02	0.40
1:G:240:THR:HA	1:G:241:PRO:HD3	1.84	0.40
1:H:256:ALA:O	1:H:312:PHE:N	2.51	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	342/344 (99%)	329 (96%)	11 (3%)	2 (1%)	25	34
1	B	342/344 (99%)	329 (96%)	11 (3%)	2 (1%)	25	34
1	C	342/344 (99%)	327 (96%)	15 (4%)	0	100	100
1	D	342/344 (99%)	329 (96%)	13 (4%)	0	100	100
1	E	342/344 (99%)	326 (95%)	15 (4%)	1 (0%)	41	51
1	F	342/344 (99%)	326 (95%)	15 (4%)	1 (0%)	41	51
1	G	342/344 (99%)	327 (96%)	14 (4%)	1 (0%)	41	51
1	H	342/344 (99%)	331 (97%)	10 (3%)	1 (0%)	41	51
All	All	2736/2752 (99%)	2624 (96%)	104 (4%)	8 (0%)	41	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	B	90	HIS
1	G	48	ALA
1	F	50	SER
1	H	48	ALA
1	B	89	PRO
1	A	322	VAL
1	E	322	VAL

5.3.2 Protein sidechains (i)

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	244/247 (99%)	233 (96%)	11 (4%)	27	37
1	B	240/247 (97%)	234 (98%)	6 (2%)	47	62
1	C	244/247 (99%)	241 (99%)	3 (1%)	71	81
1	D	245/247 (99%)	244 (100%)	1 (0%)	91	95
1	E	241/247 (98%)	238 (99%)	3 (1%)	71	81
1	F	243/247 (98%)	240 (99%)	3 (1%)	71	81
1	G	244/247 (99%)	236 (97%)	8 (3%)	38	51
1	H	234/247 (95%)	228 (97%)	6 (3%)	46	61
All	All	1935/1976 (98%)	1894 (98%)	41 (2%)	53	68

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	88	LEU
1	A	137	LEU
1	A	148	ARG
1	A	150	THR
1	A	168	PHE
1	A	230	VAL
1	A	234	ASP

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Mol	Chain	Res	Type
1	A	250	ILE
1	A	259	ARG
1	A	320	ASN
1	B	71	GLU
1	B	82	ASP
1	B	89	PRO
1	B	93	SER
1	B	135	TYR
1	B	168	PHE
1	C	88	LEU
1	C	153	ILE
1	C	168	PHE
1	D	168	PHE
1	E	96	LEU
1	E	99	GLN
1	E	168	PHE
1	F	50	SER
1	F	90	HIS
1	F	168	PHE
1	G	50	SER
1	G	73	THR
1	G	151	ARG
1	G	168	PHE
1	G	193	ARG
1	G	232	ASP
1	G	236	SER
1	G	274	HIS
1	H	49	THR
1	H	137	LEU
1	H	168	PHE
1	H	203	GLU
1	H	270	GLU
1	H	300	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	ASN
1	G	212	ASN

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 monosaccharides 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	MYI	D	402	-	12,16,16	1.53	3 (25%)	13,22,22	2.36	5 (38%)
2	MYI	A	401	-	12,16,16	1.49	3 (25%)	13,22,22	1.18	2 (15%)
2	MYI	C	402	-	12,16,16	1.68	4 (33%)	13,22,22	0.73	0
3	NAP	C	401	-	45,52,52	4.53	16 (35%)	56,80,80	2.49	6 (10%)
3	NAP	D	401	-	45,52,52	4.54	16 (35%)	56,80,80	2.48	6 (10%)
2	MYI	B	401	-	12,16,16	1.70	3 (25%)	13,22,22	1.08	2 (15%)

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	MYI	D	402	-	-	0/4/6/6	0/2/2/2
2	MYI	A	401	-	-	2/4/6/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYI	C	402	-	-	4/4/6/6	0/2/2/2
3	NAP	C	401	-	-	8/31/67/67	0/5/5/5
3	NAP	D	401	-	-	12/31/67/67	0/5/5/5
2	MYI	B	401	-	-	2/4/6/6	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAP	C2D-C1D	-16.19	1.29	1.53
3	D	401	NAP	C2D-C1D	-16.19	1.29	1.53
3	D	401	NAP	O4B-C1B	15.16	1.62	1.41
3	D	401	NAP	O4D-C1D	15.09	1.62	1.41
3	C	401	NAP	O4B-C1B	15.04	1.62	1.41
3	C	401	NAP	O4D-C1D	15.02	1.62	1.41
3	C	401	NAP	O4B-C4B	-6.39	1.30	1.45
3	D	401	NAP	O4B-C4B	-6.37	1.30	1.45
3	D	401	NAP	O4D-C4D	-6.20	1.31	1.45
3	C	401	NAP	O4D-C4D	-6.17	1.31	1.45
3	C	401	NAP	C7N-N7N	4.69	1.41	1.33
3	D	401	NAP	C7N-N7N	4.69	1.41	1.33
2	B	401	MYI	CAF-NAI	-3.63	1.29	1.36
3	C	401	NAP	P2B-O2B	3.48	1.65	1.59
3	D	401	NAP	P2B-O2B	3.44	1.65	1.59
3	D	401	NAP	C6A-N6A	3.34	1.46	1.34
3	C	401	NAP	C6A-N6A	3.33	1.46	1.34
2	C	402	MYI	CAF-NAI	-3.28	1.29	1.36
2	A	401	MYI	CAF-NAI	-3.09	1.30	1.36
3	C	401	NAP	O2D-C2D	2.98	1.50	1.43
3	D	401	NAP	O2D-C2D	2.97	1.50	1.43
2	D	402	MYI	CAO-CAN	-2.80	1.35	1.42
3	D	401	NAP	O3B-C3B	-2.67	1.36	1.43
3	C	401	NAP	O3B-C3B	-2.65	1.36	1.43
2	B	401	MYI	CAO-CAN	-2.64	1.35	1.42
2	D	402	MYI	CAF-NAI	-2.56	1.31	1.36
2	C	402	MYI	CAN-NAI	-2.55	1.30	1.38
2	C	402	MYI	CAO-CAN	-2.54	1.35	1.42
3	C	401	NAP	C3N-C7N	2.53	1.54	1.50
3	D	401	NAP	C3N-C7N	2.51	1.54	1.50
2	B	401	MYI	CAN-NAI	-2.51	1.30	1.38
3	D	401	NAP	PA-O5B	2.46	1.69	1.59
3	C	401	NAP	PA-O5B	2.46	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAP	C5A-C4A	-2.35	1.34	1.40
2	A	401	MYI	CAO-CAN	-2.35	1.36	1.42
3	D	401	NAP	C5A-C4A	-2.33	1.34	1.40
3	C	401	NAP	C5D-C4D	2.24	1.58	1.51
3	D	401	NAP	C5D-C4D	2.22	1.58	1.51
3	C	401	NAP	C5B-C4B	2.14	1.58	1.51
3	D	401	NAP	C5B-C4B	2.14	1.58	1.51
3	C	401	NAP	C2A-N3A	2.06	1.35	1.32
2	D	402	MYI	CAG-CAO	-2.06	1.38	1.42
2	A	401	MYI	CAN-NAI	-2.05	1.32	1.38
3	D	401	NAP	C2A-N3A	2.03	1.35	1.32
2	C	402	MYI	CAE-CAN	-2.02	1.38	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	NAP	C5A-C6A-N6A	13.59	141.00	120.35
3	D	401	NAP	C5A-C6A-N6A	13.56	140.96	120.35
3	C	401	NAP	N6A-C6A-N1A	-9.37	99.12	118.57
3	D	401	NAP	N6A-C6A-N1A	-9.35	99.17	118.57
3	C	401	NAP	N3A-C2A-N1A	-5.47	120.14	128.68
3	D	401	NAP	N3A-C2A-N1A	-5.42	120.21	128.68
2	D	402	MYI	CAH-CAM-CAO	-4.63	117.42	126.50
2	D	402	MYI	CAG-CAO-CAN	4.56	124.50	118.26
2	D	402	MYI	CAK-CAH-CAM	-2.90	107.97	114.71
2	B	401	MYI	CAH-CAM-CAO	2.87	132.13	126.50
3	C	401	NAP	PN-O3-PA	-2.67	123.67	132.83
3	D	401	NAP	PN-O3-PA	-2.65	123.73	132.83
2	A	401	MYI	CAK-CAH-CAM	-2.48	108.94	114.71
2	D	402	MYI	CAE-CAN-CAO	-2.40	116.38	120.76
3	C	401	NAP	C3D-C2D-C1D	2.32	104.48	100.98
3	D	401	NAP	C3D-C2D-C1D	2.29	104.42	100.98
2	D	402	MYI	OAJ-CAL-CAG	-2.23	118.35	124.43
3	D	401	NAP	C6N-N1N-C2N	-2.13	120.03	121.97
2	A	401	MYI	OAJ-CAL-CAG	-2.13	118.62	124.43
3	C	401	NAP	C6N-N1N-C2N	-2.08	120.08	121.97
2	B	401	MYI	CAA-OAJ-CAL	-2.01	113.15	117.51

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	MYI	CAK-CAH-CAM-CAF
2	B	401	MYI	CAK-CAH-CAM-CAF
2	C	402	MYI	CAK-CAH-CAM-CAF
3	C	401	NAP	C5B-O5B-PA-O3
3	C	401	NAP	C5D-O5D-PN-O1N
3	D	401	NAP	PN-O3-PA-O5B
3	D	401	NAP	C5D-O5D-PN-O1N
3	D	401	NAP	C5D-O5D-PN-O2N
3	D	401	NAP	O4D-C1D-N1N-C2N
2	C	402	MYI	CAD-CAL-OAJ-CAA
2	C	402	MYI	CAG-CAL-OAJ-CAA
3	C	401	NAP	O4B-C4B-C5B-O5B
3	D	401	NAP	O4B-C4B-C5B-O5B
2	C	402	MYI	CAK-CAH-CAM-CAO
3	D	401	NAP	C3B-C4B-C5B-O5B
3	D	401	NAP	O4D-C4D-C5D-O5D
3	D	401	NAP	C3D-C4D-C5D-O5D
3	C	401	NAP	C5D-O5D-PN-O3
3	C	401	NAP	C5B-O5B-PA-O1A
3	C	401	NAP	C5D-O5D-PN-O2N
2	A	401	MYI	CAK-CAH-CAM-CAO
3	D	401	NAP	PA-O3-PN-O1N
2	B	401	MYI	CAK-CAH-CAM-CAO
3	C	401	NAP	C2B-O2B-P2B-O3X
3	D	401	NAP	C2B-O2B-P2B-O2X
3	D	401	NAP	C5D-O5D-PN-O3
3	C	401	NAP	C5B-O5B-PA-O2A
3	D	401	NAP	C5B-O5B-PA-O2A

There are no ring outliers.

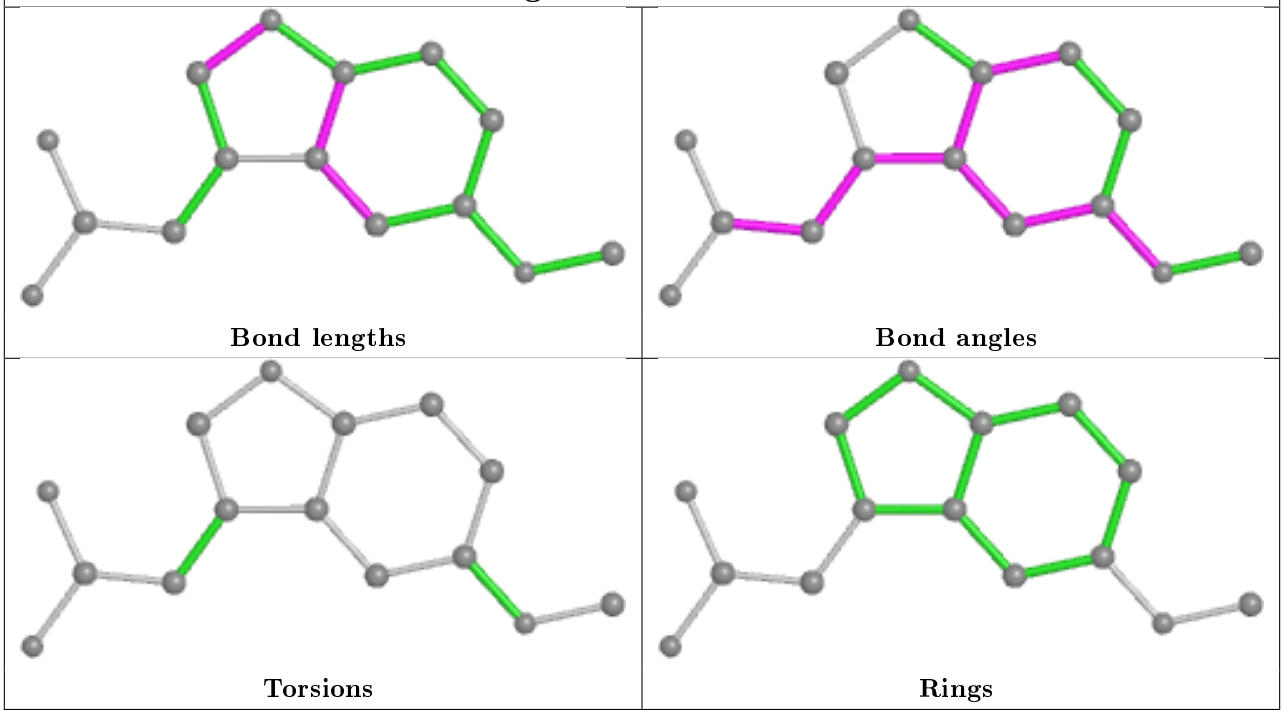
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	402	MYI	1	0
2	A	401	MYI	7	0
2	C	402	MYI	5	0
3	C	401	NAP	3	0
3	D	401	NAP	3	0
2	B	401	MYI	2	0

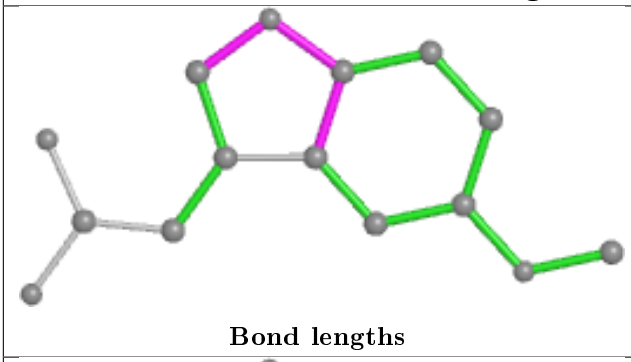
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

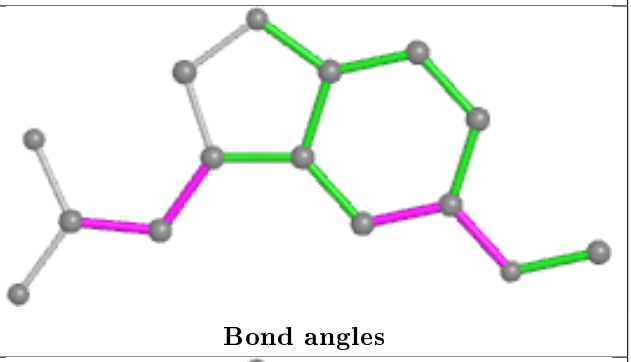
Ligand MYI D 402



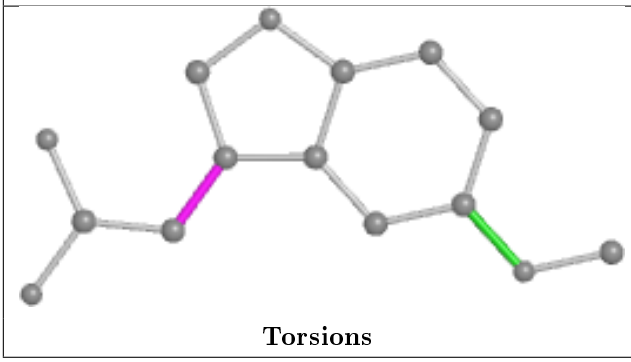
Ligand MYI A 401



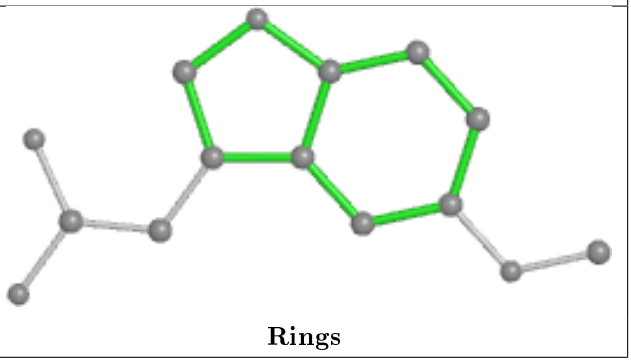
Bond lengths



Bond angles

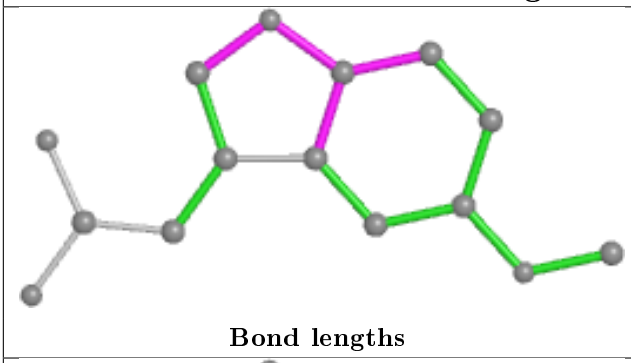


Torsions

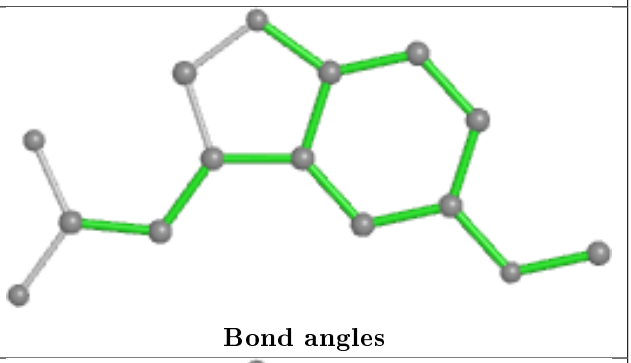


Rings

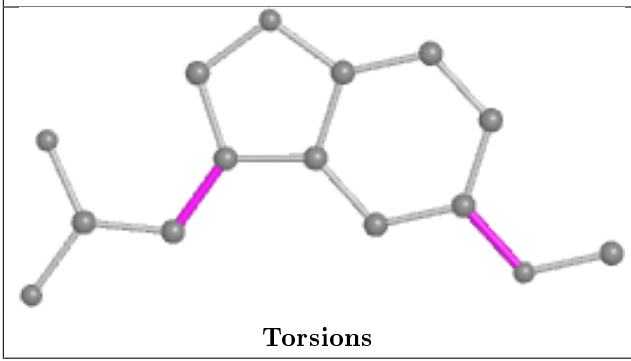
Ligand MYI C 402



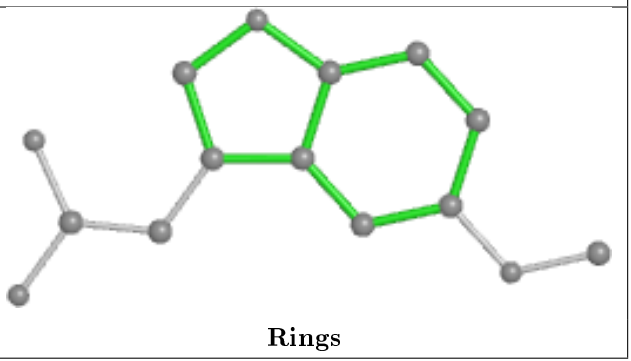
Bond lengths



Bond angles

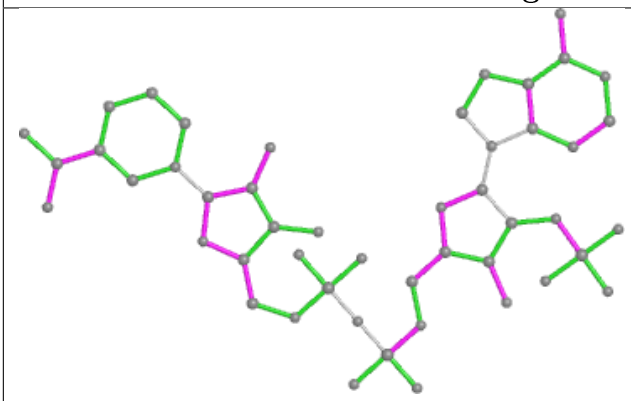


Torsions

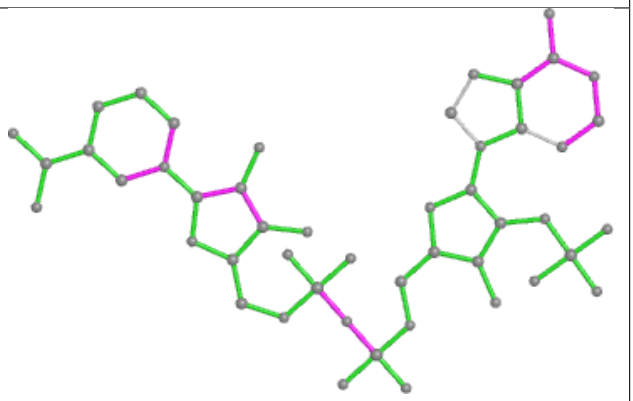


Rings

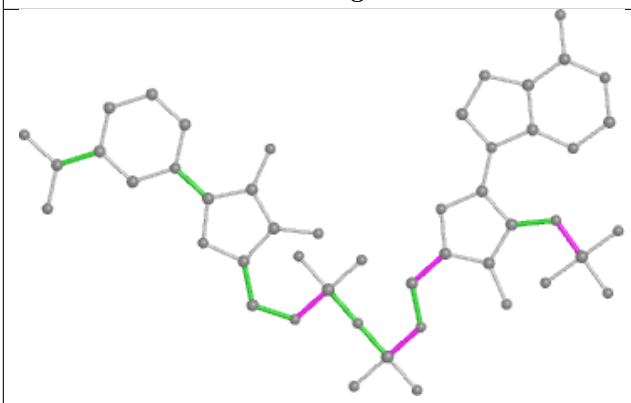
Ligand NAP C 401



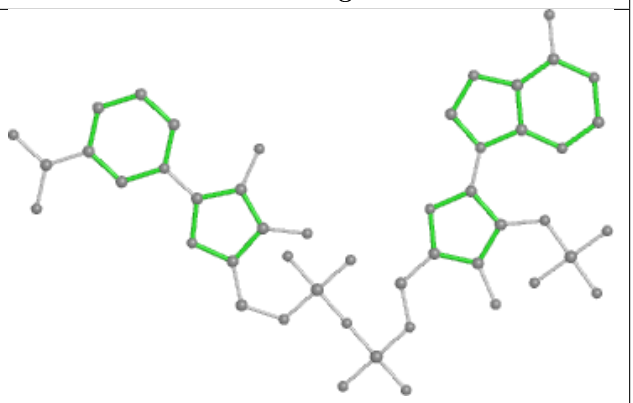
Bond lengths



Bond angles

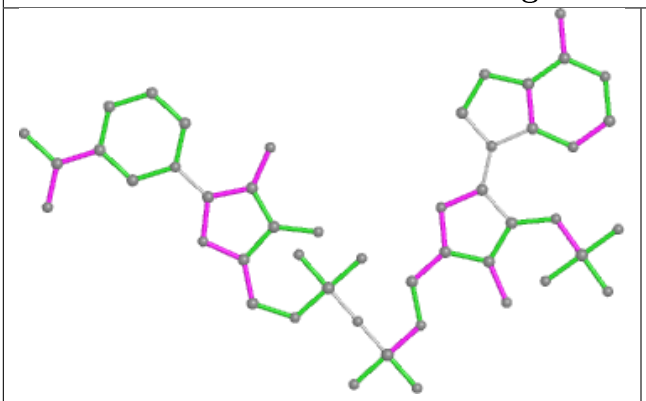


Torsions

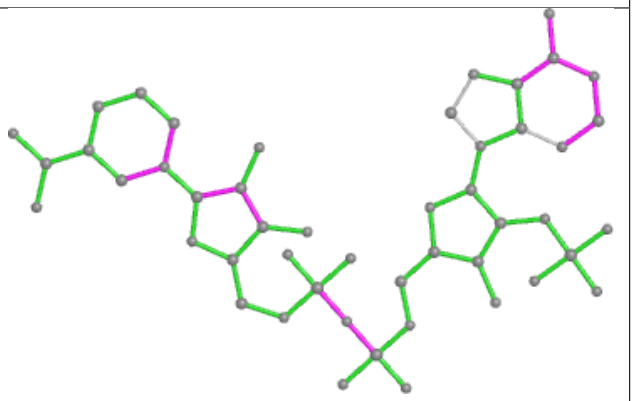


Rings

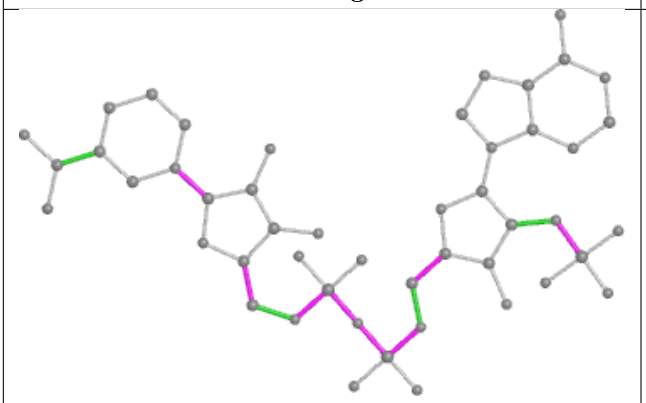
Ligand NAP D 401



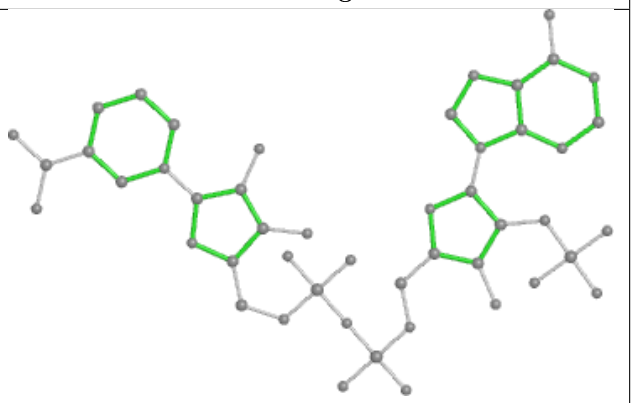
Bond lengths



Bond angles

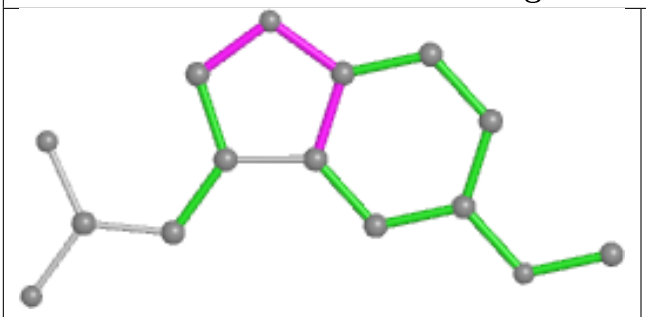


Torsions

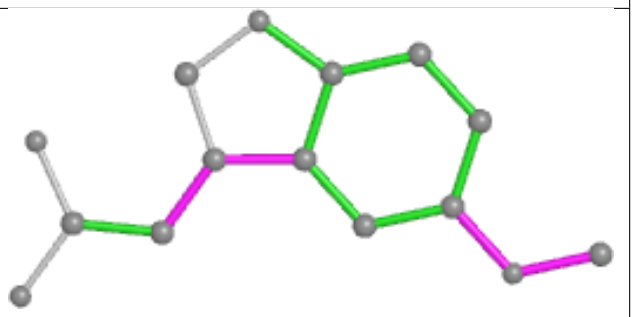


Rings

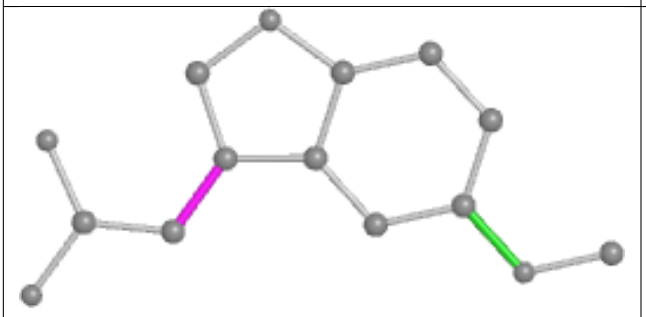
Ligand MYI B 401



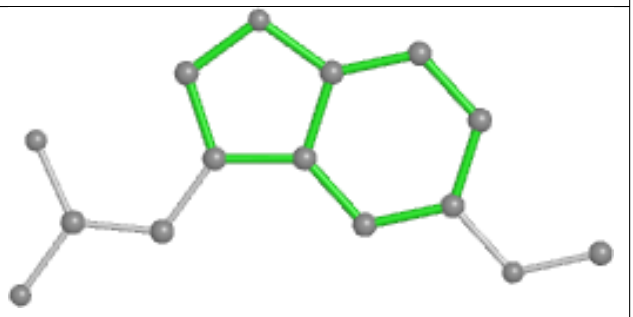
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	344/344 (100%)	0.38	8 (2%)	60	67	30, 53, 70, 89	0
1	B	344/344 (100%)	0.37	7 (2%)	65	72	40, 56, 78, 105	0
1	C	344/344 (100%)	0.32	2 (0%)	89	92	41, 54, 72, 87	0
1	D	344/344 (100%)	0.27	3 (0%)	84	88	39, 50, 65, 92	0
1	E	344/344 (100%)	0.36	11 (3%)	47	55	30, 50, 71, 92	0
1	F	344/344 (100%)	0.23	1 (0%)	94	96	38, 50, 67, 84	0
1	G	344/344 (100%)	0.35	4 (1%)	79	84	38, 52, 71, 84	0
1	H	344/344 (100%)	0.40	10 (2%)	51	59	44, 58, 78, 100	0
All	All	2752/2752 (100%)	0.33	46 (1%)	70	76	30, 53, 72, 105	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	HIS	4.0
1	A	90	HIS	3.8
1	G	175	LEU	3.6
1	A	344	GLY	3.6
1	H	180	VAL	3.5
1	H	113	PHE	3.4
1	H	91	GLY	3.0
1	H	237	VAL	2.9
1	A	9	ALA	2.8
1	G	133	TRP	2.7
1	F	158	CYS	2.6
1	D	197	THR	2.6
1	E	44	ALA	2.5
1	C	9	ALA	2.5
1	E	150	THR	2.5
1	G	134	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	40	LEU	2.5
1	H	133	TRP	2.4
1	E	178	PRO	2.4
1	A	327	GLY	2.4
1	D	311	THR	2.4
1	H	96	LEU	2.4
1	A	91	GLY	2.3
1	A	136	GLY	2.3
1	E	227	LEU	2.3
1	B	142	GLY	2.3
1	H	179	ALA	2.3
1	H	154	ALA	2.3
1	E	75	ALA	2.2
1	A	345	LEU	2.2
1	B	42	ILE	2.2
1	E	96	LEU	2.2
1	B	344	GLY	2.1
1	E	202	ALA	2.1
1	B	337	LEU	2.1
1	G	274	HIS	2.1
1	H	175	LEU	2.1
1	H	226	GLY	2.1
1	A	94	ALA	2.1
1	B	76	ALA	2.1
1	B	143	ALA	2.1
1	D	94	ALA	2.0
1	E	97	ALA	2.0
1	C	77	VAL	2.0
1	E	101	SER	2.0
1	E	175	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

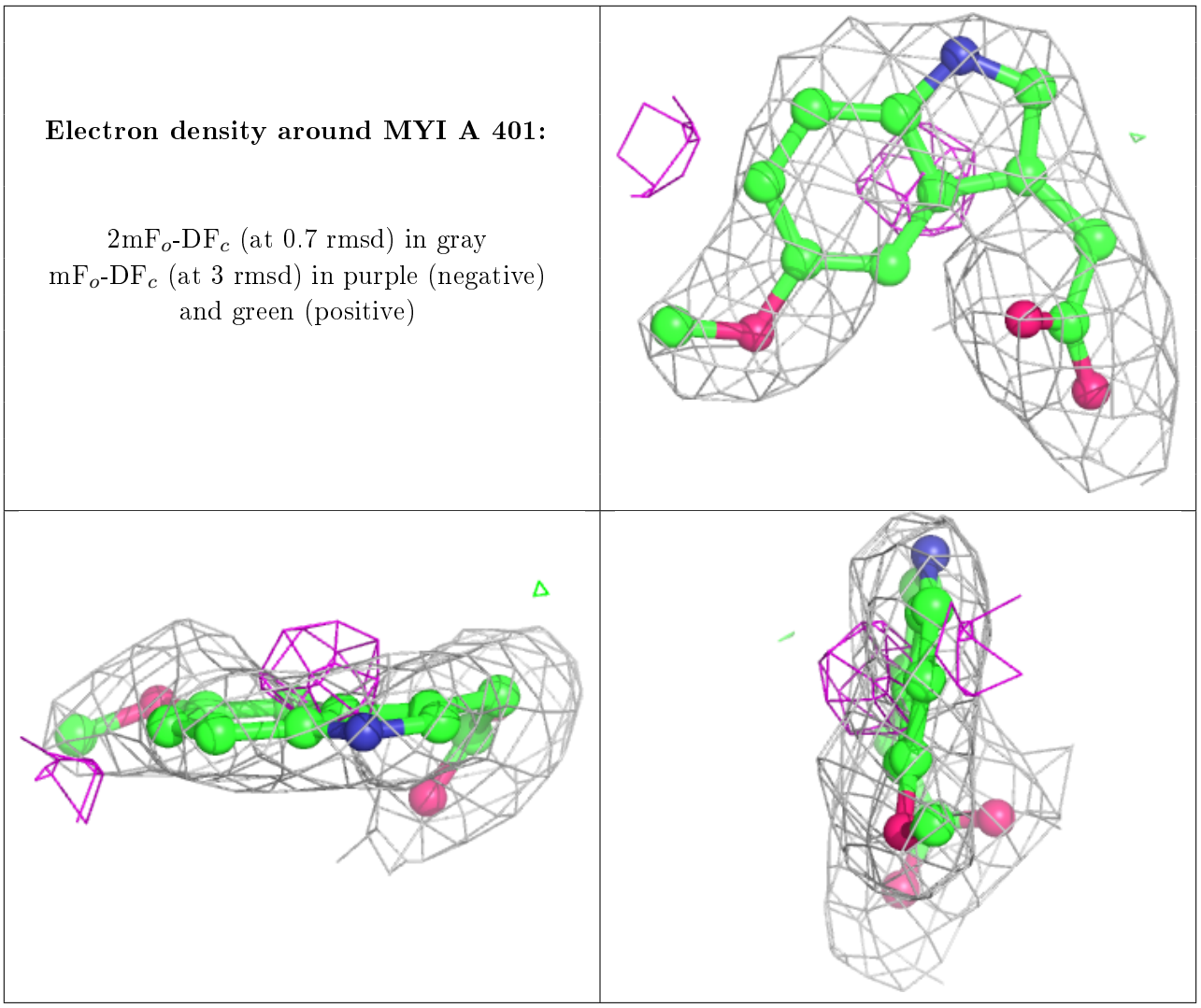
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MYI	A	401	15/15	0.83	0.26	53,58,64,67	0
2	MYI	D	402	15/15	0.84	0.21	49,57,64,69	0
2	MYI	C	402	15/15	0.86	0.25	53,57,61,64	0
2	MYI	B	401	15/15	0.92	0.15	53,59,64,64	0
3	NAP	C	401	48/48	0.93	0.15	55,65,72,75	0
3	NAP	D	401	48/48	0.94	0.17	43,56,62,64	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.

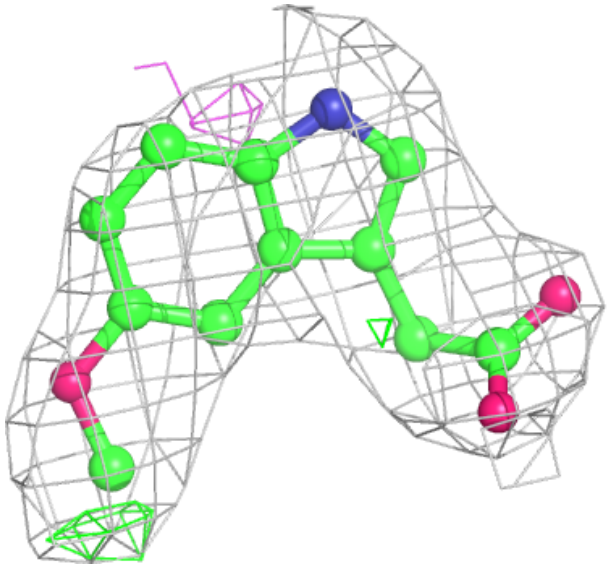
Electron density around MYI A 401:

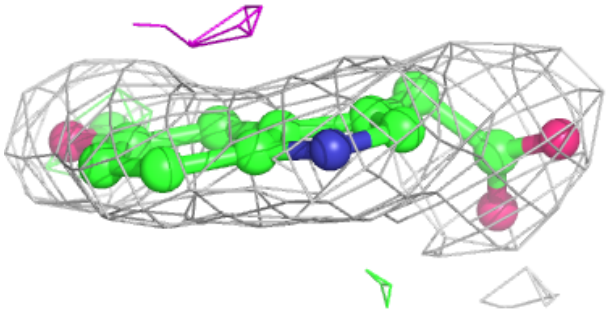
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

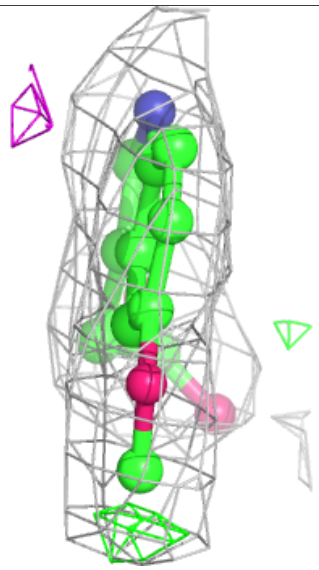


Electron density around MYI D 402:

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

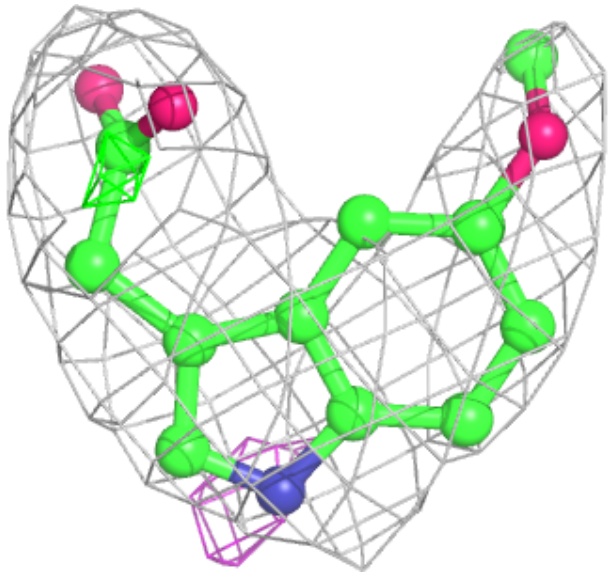


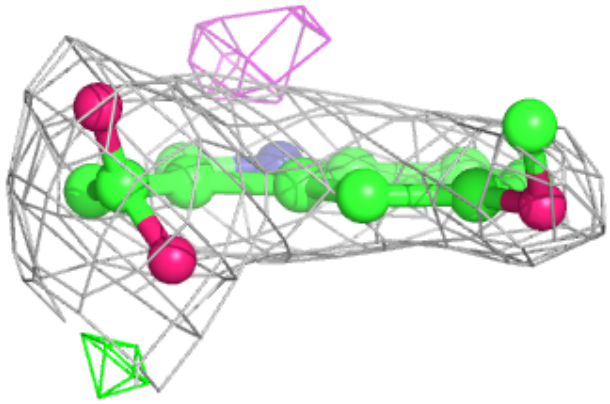


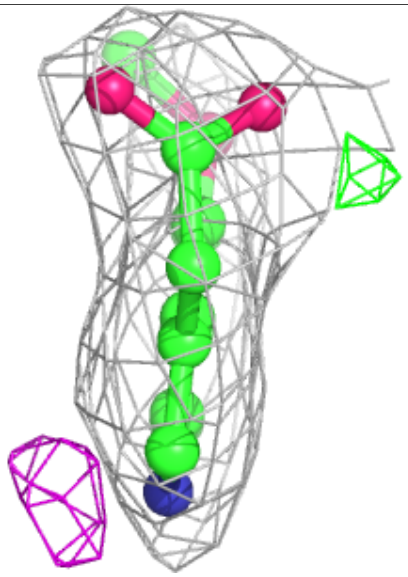


Electron density around MYI C 402:

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

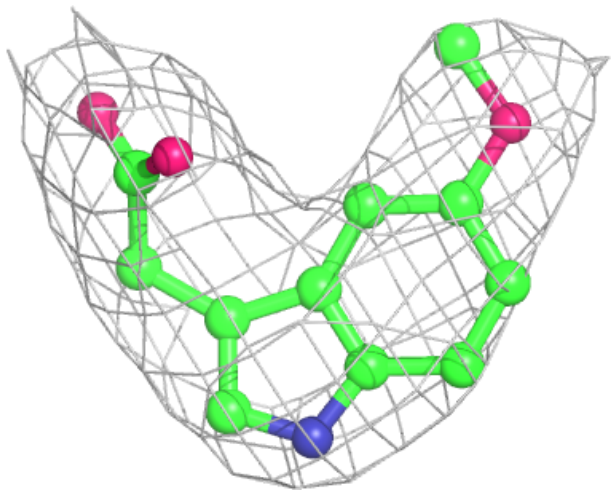


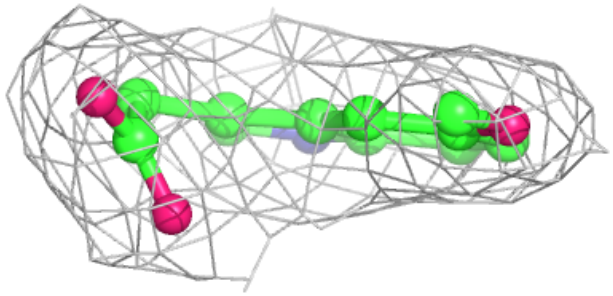


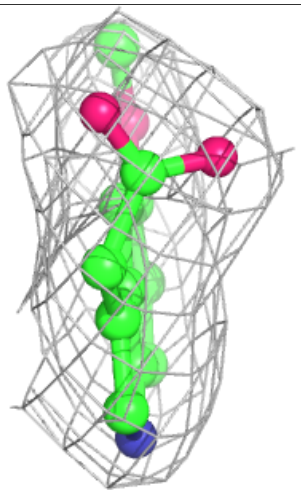


Electron density around MYI B 401:

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

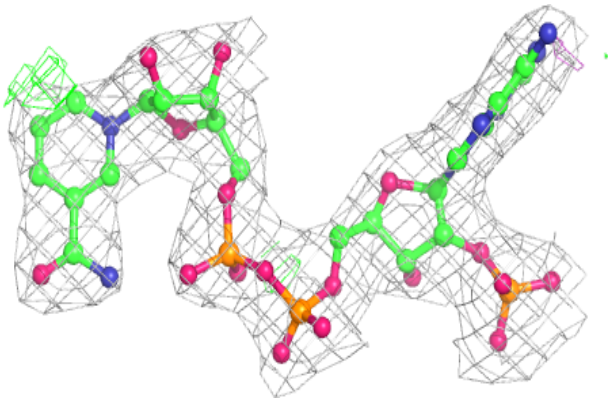


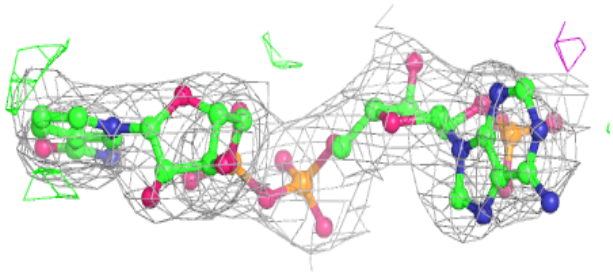


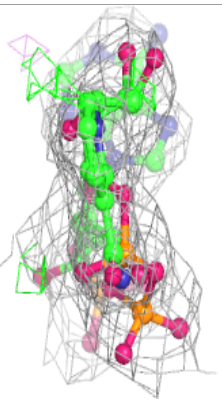


Electron density around NAP C 401:

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

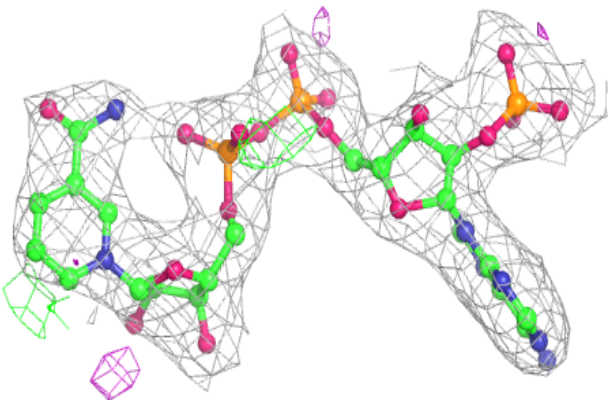


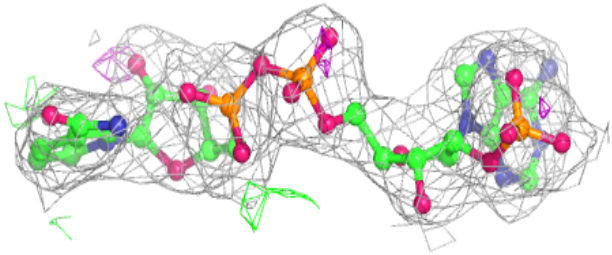


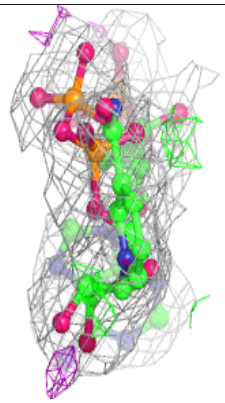


Electron density around NAP D 401:

$2mF_o$-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.