



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 06:27 AM JST

PDB ID : 7X11  
Title : Crystal structure of ME1 in complex with NADPH  
Authors : Amano, Y.  
Deposited on : 2022-02-22  
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : ?? (??), CSD ??CSD?? (????)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

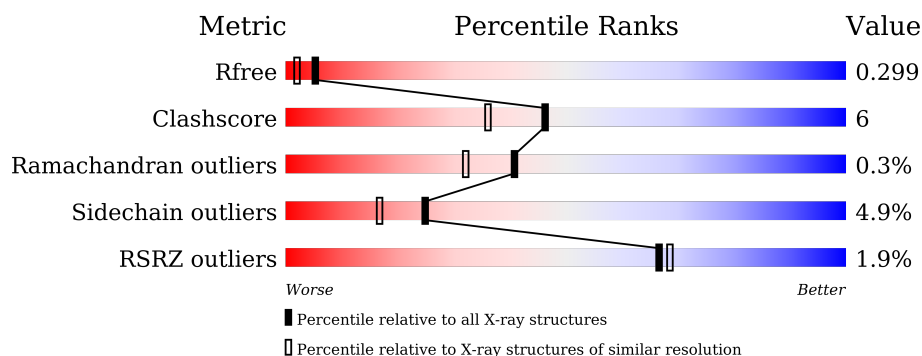
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	572	<div> <div>2%</div> <div>81% 16% ..</div> </div>
1	B	572	<div> <div>2%</div> <div>82% 16% ..</div> </div>
1	C	572	<div> <div>2%</div> <div>81% 16% ..</div> </div>
1	D	572	<div> <div>2%</div> <div>84% 13% ..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18738 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.

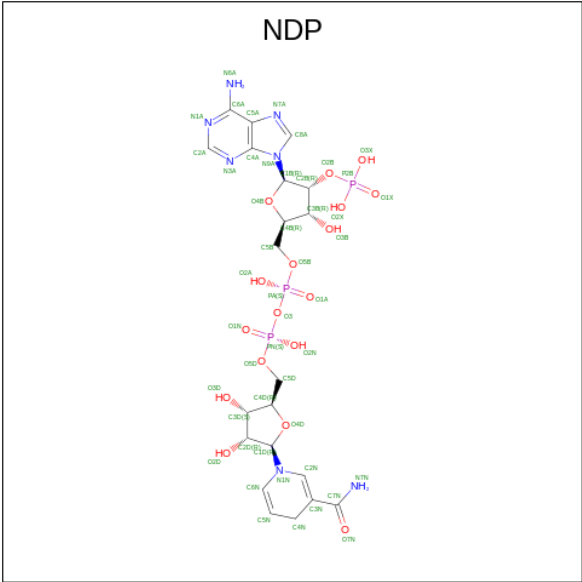
- Molecule 1 is a protein called NADP-dependent malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			
1	B	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			
1	C	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			
1	D	564	Total	C	N	O	S	0	0	0
			4451	2834	765	832	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

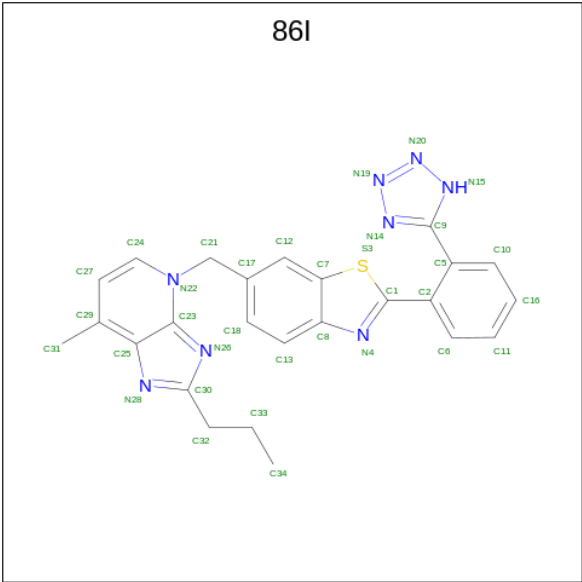
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
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 6-[(7-methyl-2-propyl-imidazo[4,5-b]pyridin-4-yl)methyl]-2-[2-(1H-1,2,3,4-tetrazol-5-yl)phenyl]-1,3-benzothiazole (three-letter code: 86I) (formula: C<sub>25</sub>H<sub>22</sub>N<sub>8</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	S	0	0
			34	25	8	1		
4	B	1	Total	C	N	S	0	0
			34	25	8	1		
4	C	1	Total	C	N	S	0	0
			34	25	8	1		
4	D	1	Total	C	N	S	0	0
			34	25	8	1		

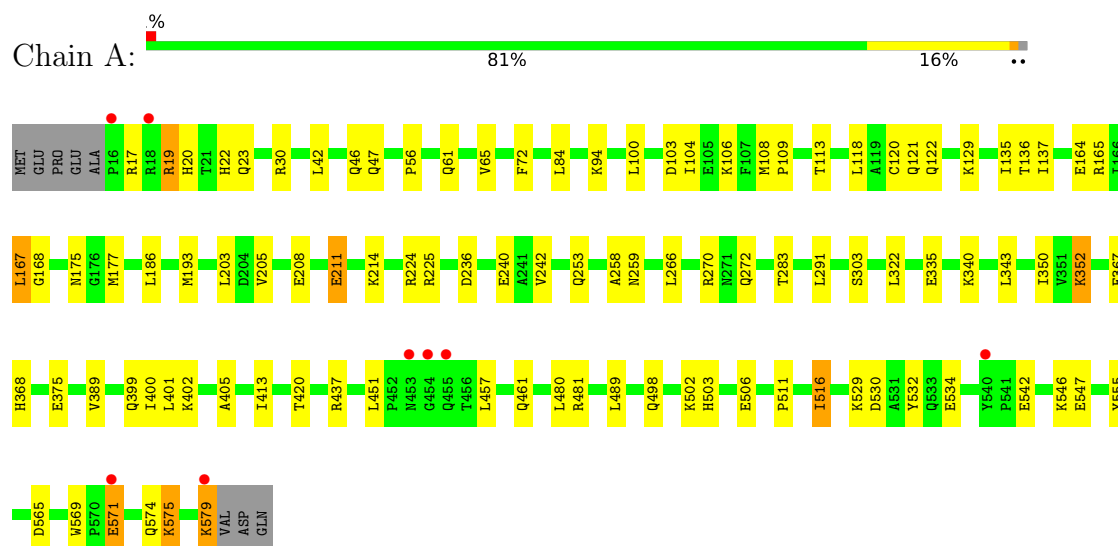
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total	O	0	0
			169	169		
5	B	200	Total	O	0	0
			200	200		
5	C	63	Total	O	0	0
			63	63		
5	D	170	Total	O	0	0
			170	170		

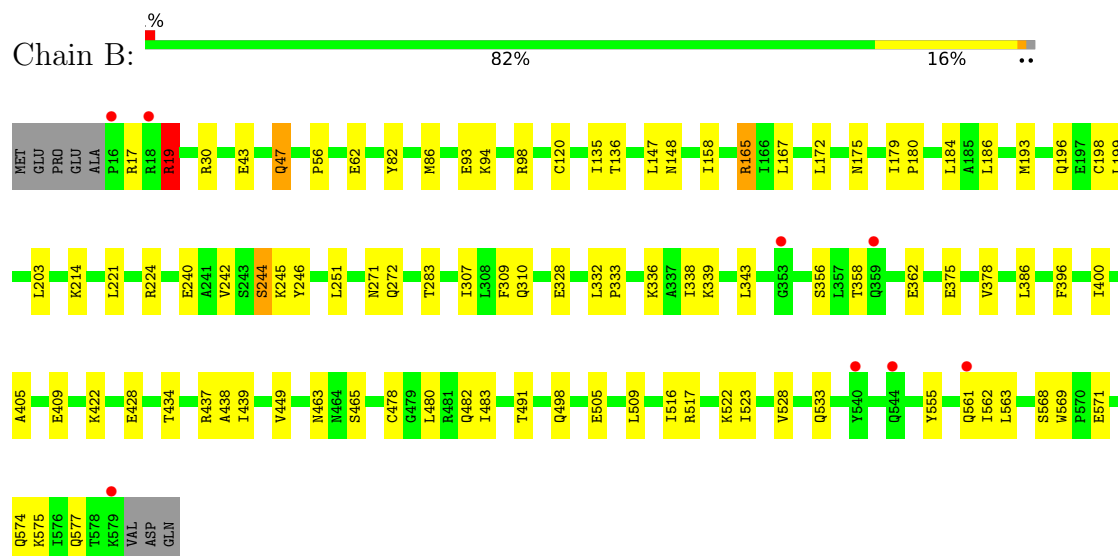
### 3 Residue-property plots [i](#)

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.

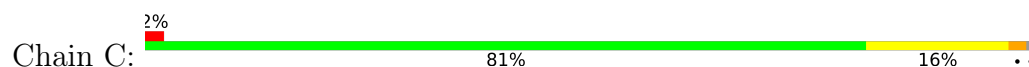
#### • Molecule 1: NADP-dependent malic enzyme

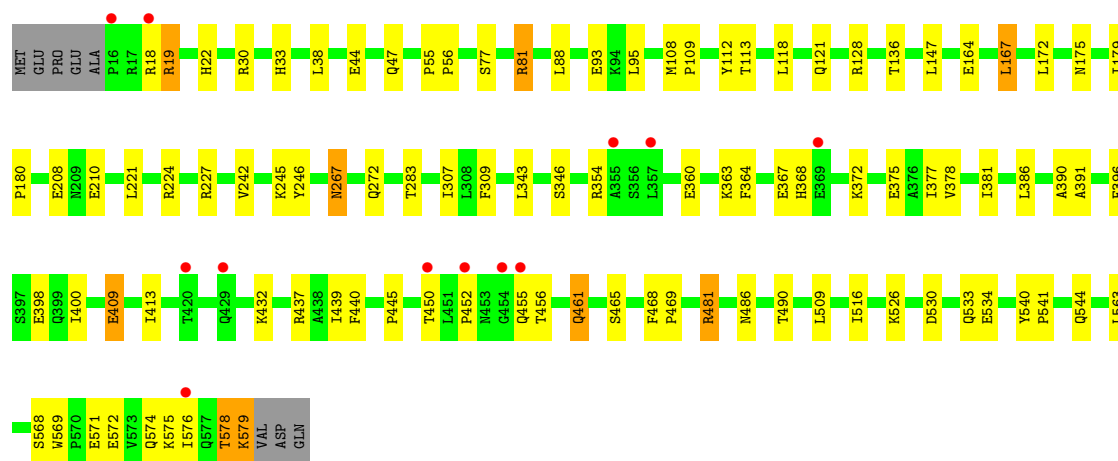


#### • Molecule 1: NADP-dependent malic enzyme

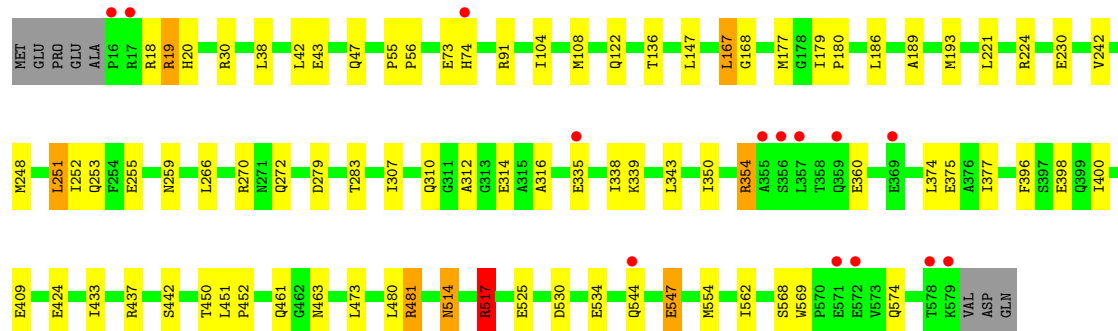
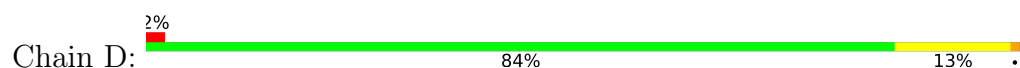


#### • Molecule 1: NADP-dependent malic enzyme





• Molecule 1: NADP-dependent malic enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.70Å 181.69Å 117.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.07 46.66 – 2.07	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.70-2.07) 93.4 (46.66-2.07)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.34 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.265 , 0.299 0.265 , 0.299	Depositor DCC
$R_{free}$ test set	8756 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	18738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 86I, MN, NDP

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	0.35	0/4538	0.72	1/6142 (0.0%)
1	B	0.36	0/4538	0.72	2/6142 (0.0%)
1	C	0.36	0/4538	0.73	2/6142 (0.0%)
1	D	0.34	0/4538	0.72	2/6142 (0.0%)
All	All	0.35	0/18152	0.72	7/24568 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	ARG	CG-CD-NE	-5.67	99.89	111.80
1	D	517	ARG	CG-CD-NE	5.36	123.06	111.80
1	B	214	LYS	CB-CA-C	-5.18	100.04	110.40
1	D	224	ARG	CG-CD-NE	-5.06	101.18	111.80
1	B	93	GLU	CB-CA-C	5.04	120.49	110.40
1	A	129	LYS	CB-CA-C	5.04	120.47	110.40
1	C	112	TYR	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	578	THR	Peptide

## 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	4451	0	4483	64	0
1	B	4451	0	4483	61	0
1	C	4451	0	4483	55	0
1	D	4451	0	4483	54	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
3	A	48	0	26	2	0
3	B	48	0	26	1	0
3	C	48	0	26	2	0
3	D	48	0	26	2	0
4	A	34	0	0	3	0
4	B	34	0	0	1	0
4	C	34	0	0	2	0
4	D	34	0	0	2	0
5	A	169	0	0	5	0
5	B	200	0	0	3	0
5	C	63	0	0	3	0
5	D	170	0	0	1	0
All	All	18738	0	18036	228	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 6.

All (228) 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:B:148:ASN:HB2	5:B:806:HOH:O	1.32	1.26
1:A:375:GLU:HA	1:A:400:ILE:HD11	1.48	0.96
1:A:375:GLU:HA	1:A:400:ILE:CD1	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD12	1:D:252:ILE:N	1.88	0.88
1:B:165:ARG:HG3	1:B:165:ARG:HH11	1.43	0.83
1:D:569:TRP:H	1:D:574:GLN:NE2	1.78	0.82
1:B:569:TRP:H	1:B:574:GLN:HE21	1.24	0.80
1:A:530:ASP:O	1:A:534:GLU:HG2	1.81	0.80
1:D:19:ARG:HG2	1:D:562:ILE:HG22	1.63	0.79
1:C:530:ASP:O	1:C:534:GLU:HG2	1.84	0.76
1:B:19:ARG:HG2	1:B:562:ILE:HG22	1.68	0.76
1:C:569:TRP:H	1:C:574:GLN:NE2	1.84	0.76
1:C:579:LYS:HB2	5:C:760:HOH:O	1.86	0.74
1:A:569:TRP:H	1:A:574:GLN:NE2	1.84	0.74
1:B:569:TRP:H	1:B:574:GLN:NE2	1.87	0.71
1:B:94:LYS:HD3	1:B:555:TYR:OH	1.91	0.70
1:A:574:GLN:HE21	1:D:42:LEU:HD23	1.58	0.69
1:B:375:GLU:HA	1:B:400:ILE:CD1	2.24	0.68
1:C:343:LEU:HD12	1:C:364:PHE:HB2	1.76	0.68
1:C:569:TRP:H	1:C:574:GLN:HE21	1.41	0.66
1:C:360:GLU:HG2	4:C:603:86I:C12	2.27	0.65
1:D:251:LEU:HD12	1:D:252:ILE:H	1.61	0.64
1:A:375:GLU:CA	1:A:400:ILE:HD11	2.27	0.63
1:C:136:THR:HB	1:C:221:LEU:HD11	1.80	0.63
1:C:450:THR:HG22	1:C:456:THR:HG23	1.81	0.62
1:C:33:HIS:CE1	1:C:93:GLU:HG2	2.35	0.61
1:C:164:GLU:OE2	1:C:227:ARG:NH2	2.30	0.61
1:D:409:GLU:O	1:D:437:ARG:HD2	1.99	0.61
1:D:248:MET:HB3	1:D:481:ARG:HH12	1.66	0.60
1:C:309:PHE:HB2	1:C:343:LEU:HD23	1.83	0.60
1:D:375:GLU:HG2	1:D:400:ILE:HG13	1.84	0.60
1:D:189:ALA:O	1:D:517:ARG:HD2	2.03	0.59
1:A:579:LYS:HE3	1:A:579:LYS:HA	1.84	0.59
1:A:303:SER:O	1:A:340:LYS:HE2	2.02	0.59
1:B:309:PHE:HB2	1:B:343:LEU:HD23	1.83	0.59
1:C:343:LEU:HD11	1:C:364:PHE:CD2	2.38	0.58
1:D:514:ASN:ND2	1:D:514:ASN:H	2.01	0.58
1:C:267:ASN:ND2	5:C:702:HOH:O	2.36	0.58
1:B:251:LEU:CD1	1:B:483:ILE:HD11	2.34	0.58
1:B:19:ARG:HH21	1:B:19:ARG:HB2	1.69	0.57
1:D:568:SER:HB2	1:D:574:GLN:HE22	1.69	0.57
1:A:529:LYS:HE3	1:A:546:LYS:HB2	1.86	0.57
1:C:439:ILE:HG22	1:C:509:LEU:HD11	1.86	0.57
1:A:481:ARG:HG2	1:A:481:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:HB2	1:A:511:PRO:HG3	1.87	0.57
1:B:465:SER:O	1:B:516:ILE:HD11	2.05	0.57
1:B:136:THR:HB	1:B:221:LEU:HD11	1.87	0.57
4:B:603:86I:C9	4:B:603:86I:S3	2.93	0.56
1:C:208:GLU:OE2	1:C:224:ARG:HD3	2.05	0.56
1:B:375:GLU:HA	1:B:400:ILE:HD11	1.86	0.56
1:D:104:ILE:O	1:D:108:MET:HB2	2.05	0.56
1:D:530:ASP:O	1:D:534:GLU:HG2	2.05	0.56
1:D:259:ASN:ND2	3:D:602:NDP:O2A	2.39	0.56
1:B:405:ALA:HB2	1:B:434:THR:HG22	1.88	0.55
1:D:525:GLU:OE2	1:D:547:GLU:HG2	2.07	0.55
1:A:571:GLU:OE2	1:A:575:LYS:HG3	2.07	0.55
1:B:120:CYS:O	1:B:175:ASN:HB3	2.07	0.55
1:C:568:SER:HB2	1:C:574:GLN:HE22	1.70	0.55
1:A:259:ASN:HB3	4:A:603:86I:C16	2.36	0.54
1:C:450:THR:HA	1:C:455:GLN:O	2.07	0.54
1:B:333:PRO:HG2	1:B:336:LYS:CG	2.37	0.54
1:A:322:LEU:HD11	1:A:489:LEU:HB2	1.89	0.54
1:D:19:ARG:CG	1:D:562:ILE:HG22	2.35	0.54
1:D:283:THR:HG23	3:D:602:NDP:H41N	1.89	0.53
1:A:574:GLN:NE2	1:D:42:LEU:HD23	2.24	0.53
1:B:62:GLU:HG3	1:B:98:ARG:NH2	2.24	0.53
1:B:358:THR:O	1:B:362:GLU:HG2	2.08	0.53
1:C:360:GLU:OE2	1:C:363:LYS:HE3	2.08	0.53
1:C:19:ARG:O	1:C:19:ARG:HG3	2.08	0.52
1:C:30:ARG:HB3	1:D:30:ARG:HB3	1.92	0.52
1:D:569:TRP:H	1:D:574:GLN:HE21	1.51	0.52
1:C:572:GLU:HB2	5:C:735:HOH:O	2.09	0.52
1:D:310:GLN:HG3	1:D:374:LEU:CD2	2.39	0.52
1:C:468:PHE:N	1:C:469:PRO:CD	2.73	0.52
1:B:378:VAL:HG21	1:B:400:ILE:HD12	1.91	0.51
1:A:109:PRO:HA	1:A:113:THR:O	2.11	0.51
1:B:165:ARG:HH11	1:B:165:ARG:CG	2.19	0.51
1:A:259:ASN:HB3	4:A:603:86I:C11	2.40	0.51
1:A:503:HIS:O	1:A:506:GLU:HB2	2.11	0.51
1:B:439:ILE:HG22	1:B:509:LEU:HD11	1.92	0.51
1:A:208:GLU:HG2	1:A:225:ARG:HG3	1.91	0.50
1:A:56:PRO:HB3	1:B:136:THR:HG21	1.93	0.50
1:C:571:GLU:O	1:C:575:LYS:HG3	2.11	0.50
1:C:386:LEU:HG	1:C:396:PHE:CZ	2.47	0.50
1:B:568:SER:HB2	1:B:574:GLN:HE22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:THR:HG23	1:C:526:LYS:HE2	1.93	0.50
1:C:377:ILE:HG23	1:C:381:ILE:HD12	1.94	0.50
1:A:574:GLN:HE21	1:D:42:LEU:CD2	2.24	0.50
1:A:502:LYS:O	1:A:506:GLU:HG3	2.12	0.49
1:B:375:GLU:HA	1:B:400:ILE:HD13	1.94	0.49
1:C:109:PRO:HA	1:C:113:THR:O	2.12	0.49
1:B:165:ARG:HG3	1:B:165:ARG:NH1	2.19	0.49
1:C:283:THR:HG23	3:C:602:NDP:H41N	1.92	0.49
1:B:251:LEU:HD12	1:B:483:ILE:HD11	1.94	0.49
1:A:94:LYS:HD3	1:A:555:TYR:OH	2.12	0.49
1:B:386:LEU:HG	1:B:396:PHE:CZ	2.48	0.49
1:A:61:GLN:O	1:A:65:VAL:HG23	2.13	0.49
1:A:283:THR:HG23	3:A:602:NDP:H41N	1.95	0.48
1:A:532:TYR:CD1	1:A:542:GLU:HG3	2.48	0.48
1:B:478:CYS:HB3	1:B:528:VAL:HG22	1.95	0.48
1:B:517:ARG:HG2	5:B:828:HOH:O	2.12	0.48
1:B:498:GLN:OE1	1:B:522:LYS:HD2	2.12	0.48
1:A:30:ARG:HB3	1:B:30:ARG:HB3	1.95	0.48
1:A:120:CYS:O	1:A:175:ASN:HB3	2.14	0.48
1:C:481:ARG:HH11	1:C:481:ARG:HB3	1.78	0.48
1:D:442:SER:O	1:D:461:GLN:HA	2.13	0.48
1:A:118:LEU:HA	1:A:121:GLN:HE21	1.77	0.48
1:A:136:THR:HG21	1:B:56:PRO:HB3	1.96	0.48
1:C:468:PHE:N	1:C:469:PRO:HD3	2.28	0.48
1:D:248:MET:CB	1:D:481:ARG:HH12	2.26	0.48
1:D:91:ARG:HG3	1:D:91:ARG:HH11	1.79	0.47
1:A:214:LYS:HB3	5:A:770:HOH:O	2.14	0.47
1:B:333:PRO:HG2	1:B:336:LYS:HG2	1.96	0.47
1:A:451:LEU:HD11	1:A:457:LEU:HD11	1.96	0.47
1:C:346:SER:HB2	3:C:602:NDP:O2X	2.15	0.47
1:B:19:ARG:NH1	1:B:196:GLN:HE22	2.12	0.47
1:C:578:THR:O	1:C:579:LYS:HB3	2.13	0.47
1:D:136:THR:HB	1:D:221:LEU:HD11	1.96	0.47
1:D:251:LEU:HD12	1:D:251:LEU:C	2.32	0.46
1:A:193:MET:HE3	1:A:193:MET:HB2	1.73	0.46
1:D:310:GLN:HG3	1:D:374:LEU:HD22	1.97	0.46
4:D:603:86I:C9	4:D:603:86I:S3	3.04	0.46
1:B:184:LEU:HD13	1:B:198:CYS:HB3	1.98	0.46
1:B:405:ALA:O	1:B:437:ARG:NH2	2.48	0.45
1:B:165:ARG:CG	1:B:165:ARG:NH1	2.79	0.45
1:A:42:LEU:O	1:A:46:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLU:HA	1:C:563:LEU:HD21	1.98	0.45
1:A:17:ARG:NH1	5:A:703:HOH:O	2.49	0.45
1:B:19:ARG:O	1:B:562:ILE:HA	2.16	0.45
1:C:172:LEU:O	1:C:175:ASN:HB2	2.17	0.45
1:B:17:ARG:HE	1:B:17:ARG:HB3	1.56	0.45
1:B:375:GLU:HG3	5:B:890:HOH:O	2.17	0.45
4:A:603:86I:S3	4:A:603:86I:C9	3.04	0.44
1:A:516:ILE:O	1:A:516:ILE:HD12	2.16	0.44
1:A:137:ILE:HB	1:A:205:VAL:HG12	1.98	0.44
1:D:451:LEU:HB3	1:D:452:PRO:CD	2.48	0.44
1:A:42:LEU:HD23	1:D:574:GLN:HE21	1.82	0.44
1:A:266:LEU:O	1:A:270:ARG:HB3	2.18	0.44
1:D:177:MET:O	1:D:180:PRO:HD2	2.18	0.44
1:A:211:GLU:H	1:A:211:GLU:HG2	1.51	0.44
1:A:401:LEU:HD23	1:A:413:ILE:HD13	1.99	0.44
1:B:434:THR:HG21	1:B:438:ALA:HB2	1.99	0.44
1:D:19:ARG:NH2	1:D:19:ARG:HB2	2.32	0.44
1:D:461:GLN:HG3	1:D:463:ASN:HB2	2.00	0.44
1:B:179:ILE:HB	1:B:180:PRO:HD3	2.00	0.44
1:B:575:LYS:HE3	1:B:577:GLN:HA	2.00	0.44
1:C:367:GLU:O	1:C:368:HIS:HB2	2.18	0.44
1:A:23:GLN:NE2	5:A:705:HOH:O	2.51	0.44
1:D:167:LEU:HB3	1:D:168:GLY:H	1.53	0.44
1:B:135:ILE:O	1:B:203:LEU:HA	2.17	0.43
1:B:491:THR:HG23	1:B:523:ILE:HG12	2.00	0.43
1:D:19:ARG:HB2	1:D:19:ARG:HH21	1.82	0.43
1:A:165:ARG:NH2	3:A:602:NDP:O1A	2.51	0.43
1:A:352:LYS:HG3	5:A:706:HOH:O	2.18	0.43
1:B:82:TYR:O	1:B:86:MET:HG2	2.18	0.43
1:D:179:ILE:HB	1:D:180:PRO:HD3	2.00	0.43
1:B:148:ASN:ND2	1:D:20:HIS:HB2	2.33	0.43
1:A:72:PHE:CE1	1:A:106:LYS:HE2	2.54	0.43
1:D:193:MET:HE3	1:D:193:MET:HB2	1.82	0.43
1:D:312:ALA:HA	1:D:316:ALA:HB3	2.00	0.43
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.84	0.43
1:C:38:LEU:HD21	1:C:55:PRO:HG2	2.00	0.43
1:A:167:LEU:HB3	1:A:168:GLY:H	1.56	0.43
1:A:104:ILE:O	1:A:108:MET:HG3	2.18	0.43
1:B:193:MET:HE3	1:B:193:MET:HB2	1.88	0.43
1:C:108:MET:N	1:C:109:PRO:HD2	2.34	0.43
1:A:367:GLU:O	1:A:368:HIS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:HG2	1:B:562:ILE:CG2	2.44	0.43
1:C:88:LEU:HD11	1:C:95:LEU:HD23	2.01	0.43
1:D:266:LEU:O	1:D:270:ARG:HB3	2.19	0.42
1:B:283:THR:HG23	3:B:602:NDP:H41N	2.01	0.42
1:D:253:GLN:NE2	1:D:255:GLU:OE1	2.51	0.42
1:B:328:GLU:HA	1:B:332:LEU:O	2.20	0.42
1:C:118:LEU:HA	1:C:121:GLN:HE21	1.84	0.42
1:C:534:GLU:HG2	1:C:534:GLU:H	1.74	0.42
1:C:465:SER:O	1:C:516:ILE:HD11	2.19	0.42
1:D:193:MET:HE1	1:D:473:LEU:HA	2.02	0.42
1:D:360:GLU:HG2	4:D:603:86I:S3	2.59	0.42
1:B:172:LEU:O	1:B:175:ASN:HB2	2.19	0.42
1:C:245:LYS:HE3	1:C:246:TYR:CE1	2.54	0.42
1:D:354:ARG:HE	1:D:354:ARG:HB3	1.60	0.42
1:B:480:LEU:HD12	1:B:480:LEU:HA	1.93	0.42
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.91	0.42
1:D:279:ASP:HB3	1:D:314:GLU:OE2	2.20	0.42
1:B:271:ASN:O	1:B:482:GLN:NE2	2.48	0.42
1:B:240:GLU:O	1:B:244:SER:HB3	2.19	0.42
1:C:113:THR:CG2	1:C:167:LEU:HD11	2.50	0.42
1:D:554:MET:O	5:D:701:HOH:O	2.22	0.41
1:D:19:ARG:HH21	1:D:19:ARG:CB	2.32	0.41
1:D:38:LEU:HD21	1:D:55:PRO:HG2	2.01	0.41
1:D:398:GLU:HG3	1:D:433:ILE:HG12	2.02	0.41
1:C:56:PRO:HB3	1:D:136:THR:HG21	2.03	0.41
1:A:343:LEU:CB	1:A:350:ILE:HD12	2.51	0.41
1:B:463:ASN:OD1	1:B:465:SER:HB2	2.20	0.41
1:C:375:GLU:HA	1:C:400:ILE:CD1	2.51	0.41
1:C:413:ILE:O	1:C:440:PHE:HA	2.20	0.41
1:A:405:ALA:O	1:A:437:ARG:NH2	2.53	0.41
1:B:428:GLU:OE2	1:B:449:VAL:HG13	2.20	0.41
1:C:576:ILE:HD12	1:C:576:ILE:H	1.86	0.41
1:C:576:ILE:HD12	1:C:576:ILE:N	2.36	0.41
4:C:603:86I:C9	4:C:603:86I:S3	3.08	0.41
1:D:374:LEU:HA	1:D:377:ILE:HD12	2.03	0.41
1:D:396:PHE:CG	1:D:424:GLU:HB3	2.55	0.41
1:A:399:GLN:NE2	5:A:709:HOH:O	2.53	0.41
1:C:540:TYR:HA	1:C:541:PRO:C	2.40	0.41
1:A:19:ARG:CG	1:A:19:ARG:O	2.68	0.41
1:A:236:ASP:O	1:A:240:GLU:HG3	2.19	0.41
1:B:245:LYS:HE3	1:B:246:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:O	1:A:203:LEU:HA	2.21	0.41
1:C:390:ALA:O	1:C:391:ALA:HB3	2.20	0.41
1:C:450:THR:HG22	1:C:456:THR:CG2	2.48	0.41
1:D:343:LEU:HB2	1:D:350:ILE:HD12	2.03	0.41
1:A:113:THR:HG22	1:A:167:LEU:HD21	2.03	0.41
1:A:481:ARG:HG2	1:A:481:ARG:NH1	2.35	0.41
1:A:579:LYS:HA	1:A:579:LYS:CE	2.51	0.41
1:A:402:LYS:HE2	1:A:402:LYS:HB3	1.89	0.40
1:C:378:VAL:HG21	1:C:400:ILE:HG23	2.03	0.40
1:A:164:GLU:HG2	1:A:258:ALA:HB2	2.02	0.40
1:B:62:GLU:HG3	1:B:98:ARG:HH22	1.84	0.40
1:A:569:TRP:H	1:A:574:GLN:HE21	1.67	0.40
1:C:77:SER:O	1:C:81:ARG:HD2	2.22	0.40
1:C:179:ILE:HB	1:C:180:PRO:HD3	2.02	0.40
1:C:445:PRO:HG3	1:C:461:GLN:NE2	2.36	0.40
1:A:208:GLU:OE2	1:A:224:ARG:NH1	2.47	0.40
1:B:158:ILE:HG12	1:B:199:LEU:HB3	2.04	0.40
1:A:20:HIS:CE1	1:A:565:ASP:HB2	2.57	0.40
1:B:43:GLU:O	1:B:47:GLN:HB2	2.21	0.40
1:D:525:GLU:CD	1:D:547:GLU:HG2	2.42	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	562/572 (98%)	546 (97%)	14 (2%)	2 (0%)	34	25
1	B	562/572 (98%)	543 (97%)	18 (3%)	1 (0%)	47	39
1	C	562/572 (98%)	544 (97%)	15 (3%)	3 (0%)	29	19
1	D	562/572 (98%)	548 (98%)	14 (2%)	0	100	100
All	All	2248/2288 (98%)	2181 (97%)	61 (3%)	6 (0%)	41	32



All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ARG
1	A	103	ASP
1	C	398	GLU
1	C	409	GLU
1	A	389	VAL
1	C	452	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/490 (99%)	460 (95%)	23 (5%)	25	18
1	B	483/490 (99%)	461 (95%)	22 (5%)	27	19
1	C	483/490 (99%)	460 (95%)	23 (5%)	25	18
1	D	483/490 (99%)	456 (94%)	27 (6%)	21	13
All	All	1932/1960 (99%)	1837 (95%)	95 (5%)	25	17

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	22	HIS
1	A	47	GLN
1	A	84	LEU
1	A	100	LEU
1	A	122	GLN
1	A	167	LEU
1	A	177	MET
1	A	186	LEU
1	A	211	GLU
1	A	242	VAL
1	A	253	GLN
1	A	272	GLN
1	A	335	GLU

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Mol	Chain	Res	Type
1	A	352	LYS
1	A	420	THR
1	A	461	GLN
1	A	480	LEU
1	A	516	ILE
1	A	547	GLU
1	A	571	GLU
1	A	575	LYS
1	A	579	LYS
1	B	19	ARG
1	B	47	GLN
1	B	147	LEU
1	B	165	ARG
1	B	167	LEU
1	B	186	LEU
1	B	224	ARG
1	B	242	VAL
1	B	244	SER
1	B	272	GLN
1	B	307	ILE
1	B	310	GLN
1	B	338	ILE
1	B	339	LYS
1	B	356	SER
1	B	409	GLU
1	B	422	LYS
1	B	505	GLU
1	B	533	GLN
1	B	561	GLN
1	B	563	LEU
1	B	571	GLU
1	C	18	ARG
1	C	19	ARG
1	C	22	HIS
1	C	47	GLN
1	C	128	ARG
1	C	147	LEU
1	C	167	LEU
1	C	210	GLU
1	C	242	VAL
1	C	267	ASN
1	C	272	GLN

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Mol	Chain	Res	Type
1	C	307	ILE
1	C	354	ARG
1	C	372	LYS
1	C	409	GLU
1	C	432	LYS
1	C	437	ARG
1	C	461	GLN
1	C	481	ARG
1	C	486	ASN
1	C	533	GLN
1	C	544	GLN
1	C	579	LYS
1	D	18	ARG
1	D	19	ARG
1	D	43	GLU
1	D	47	GLN
1	D	56	PRO
1	D	73	GLU
1	D	74	HIS
1	D	122	GLN
1	D	147	LEU
1	D	167	LEU
1	D	186	LEU
1	D	230	GLU
1	D	242	VAL
1	D	251	LEU
1	D	272	GLN
1	D	307	ILE
1	D	335	GLU
1	D	338	ILE
1	D	339	LYS
1	D	354	ARG
1	D	450	THR
1	D	480	LEU
1	D	481	ARG
1	D	514	ASN
1	D	517	ARG
1	D	544	GLN
1	D	547	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	23	GLN
1	A	33	HIS
1	A	49	ASN
1	A	76	ASN
1	A	121	GLN
1	A	196	GLN
1	A	455	GLN
1	A	461	GLN
1	A	561	GLN
1	A	574	GLN
1	B	22	HIS
1	B	76	ASN
1	B	121	GLN
1	B	310	GLN
1	B	574	GLN
1	C	33	HIS
1	C	49	ASN
1	C	121	GLN
1	C	196	GLN
1	C	267	ASN
1	C	321	HIS
1	C	455	GLN
1	C	461	GLN
1	C	533	GLN
1	C	574	GLN
1	D	76	ASN
1	D	399	GLN
1	D	514	ASN
1	D	561	GLN
1	D	574	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

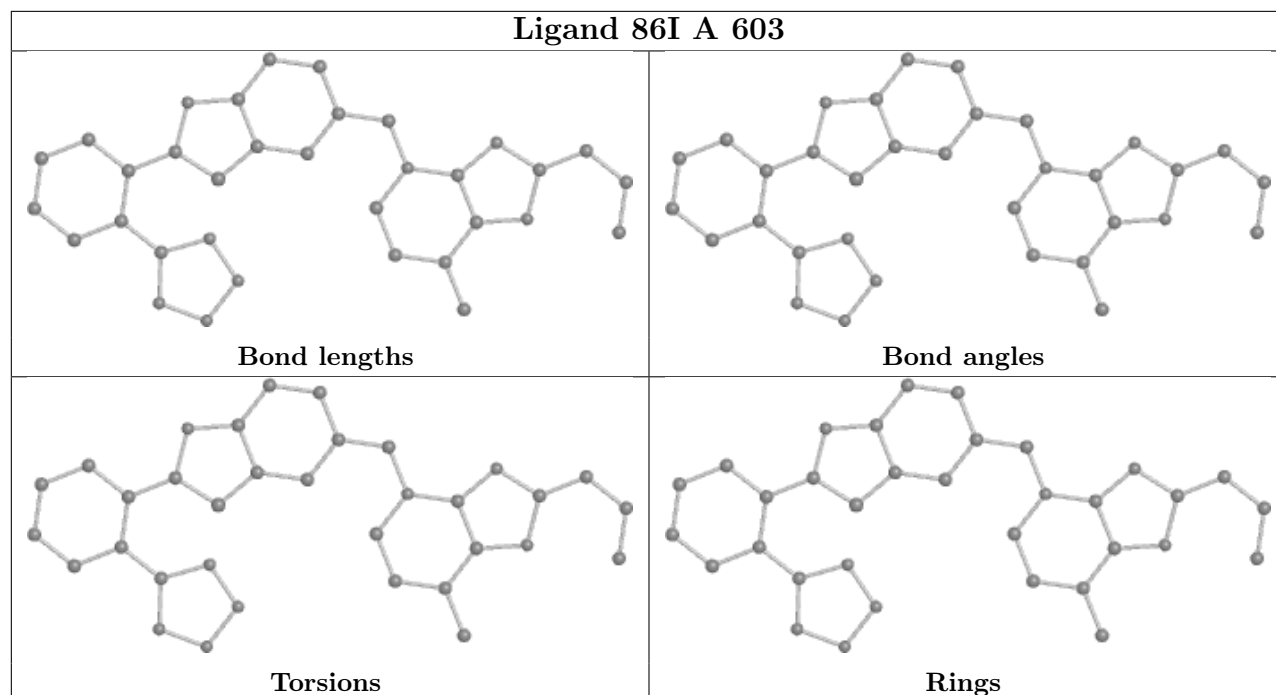
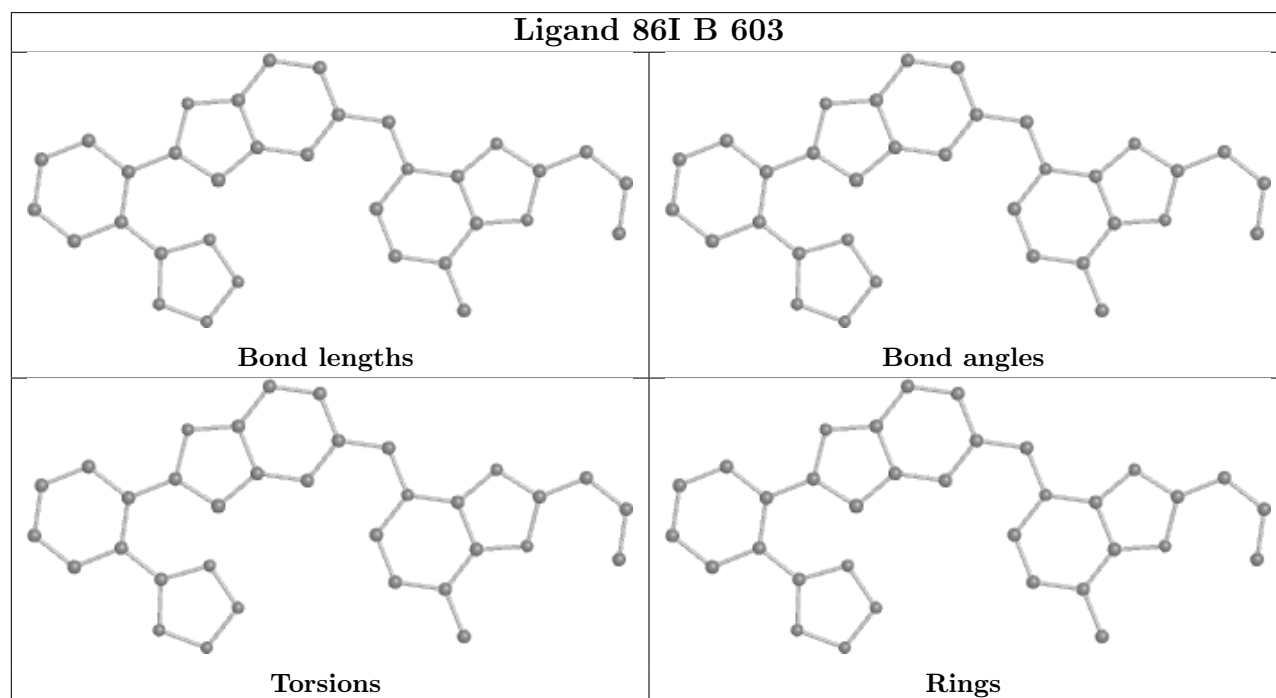
There are no chirality outliers.

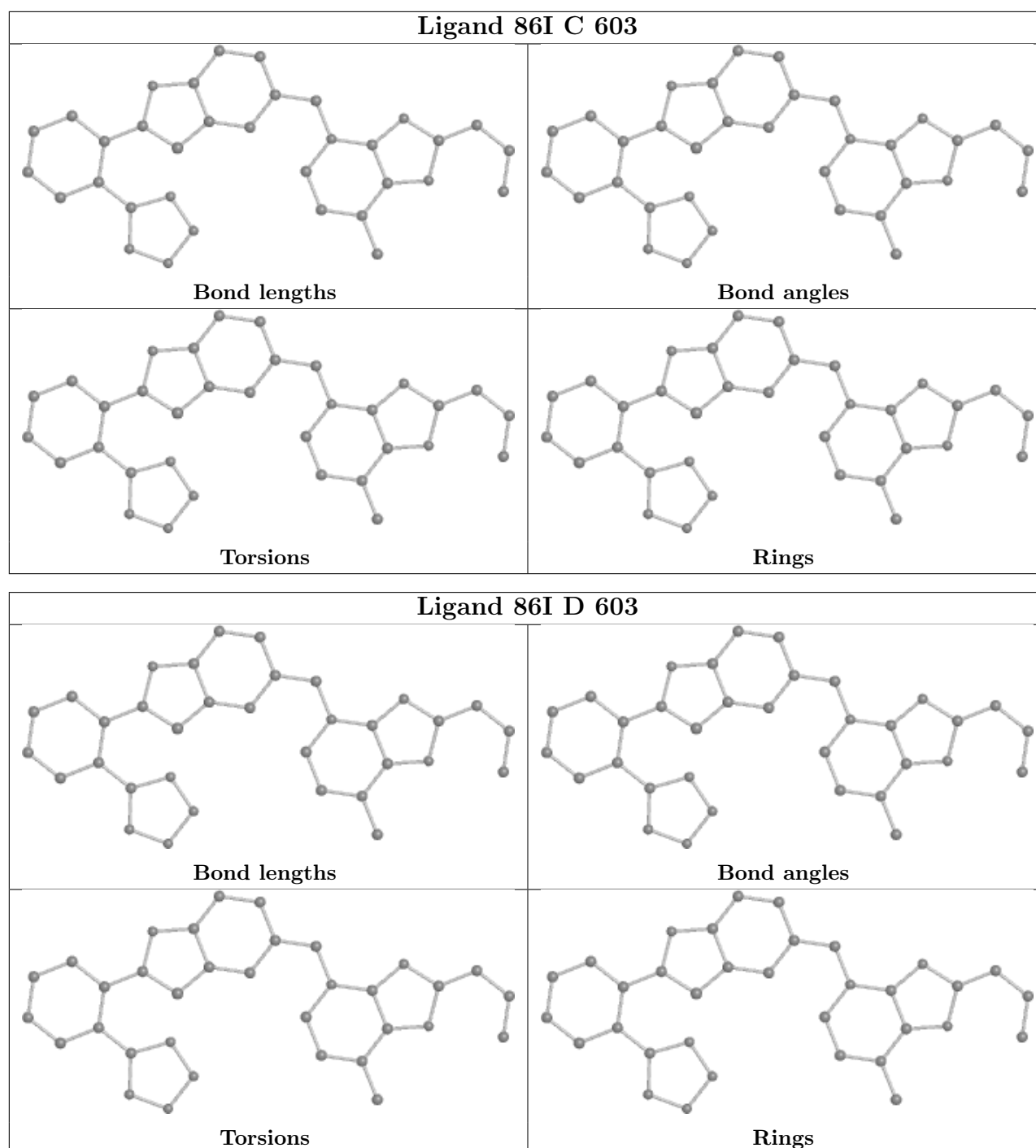
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

**Ligand 86I A 603****Ligand 86I B 603**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	564/572 (98%)	0.10	8 (1%) 75 76	20, 32, 51, 88	0
1	B	564/572 (98%)	0.11	8 (1%) 75 76	19, 31, 53, 81	0
1	C	564/572 (98%)	0.14	12 (2%) 63 65	19, 32, 57, 99	0
1	D	564/572 (98%)	0.14	14 (2%) 57 60	20, 32, 57, 94	0
All	All	2256/2288 (98%)	0.13	42 (1%) 66 68	19, 32, 56, 99	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	GLY	7.6
1	D	16	PRO	6.9
1	C	355	ALA	4.7
1	A	16	PRO	4.5
1	C	452	PRO	3.9
1	A	579	LYS	3.7
1	B	579	LYS	3.7
1	D	579	LYS	3.4
1	B	16	PRO	3.2
1	D	356	SER	3.1
1	D	359	GLN	3.0
1	D	357	LEU	2.9
1	C	369	GLU	2.9
1	A	453	ASN	2.8
1	A	455	GLN	2.8
1	C	576	ILE	2.8
1	C	18	ARG	2.8
1	D	572	GLU	2.7
1	D	355	ALA	2.7
1	B	544	GLN	2.7
1	A	18	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	544	GLN	2.6
1	C	16	PRO	2.5
1	C	429	GLN	2.5
1	D	571	GLU	2.4
1	C	357	LEU	2.4
1	B	561	GLN	2.3
1	D	17	ARG	2.3
1	D	369	GLU	2.3
1	B	18	ARG	2.3
1	D	578	THR	2.2
1	C	420	THR	2.1
1	D	74	HIS	2.1
1	A	540	TYR	2.1
1	D	335	GLU	2.1
1	B	540	TYR	2.1
1	A	571	GLU	2.0
1	C	455	GLN	2.0
1	A	454	GLY	2.0
1	B	353	GLY	2.0
1	B	359	GLN	2.0
1	C	450	THR	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

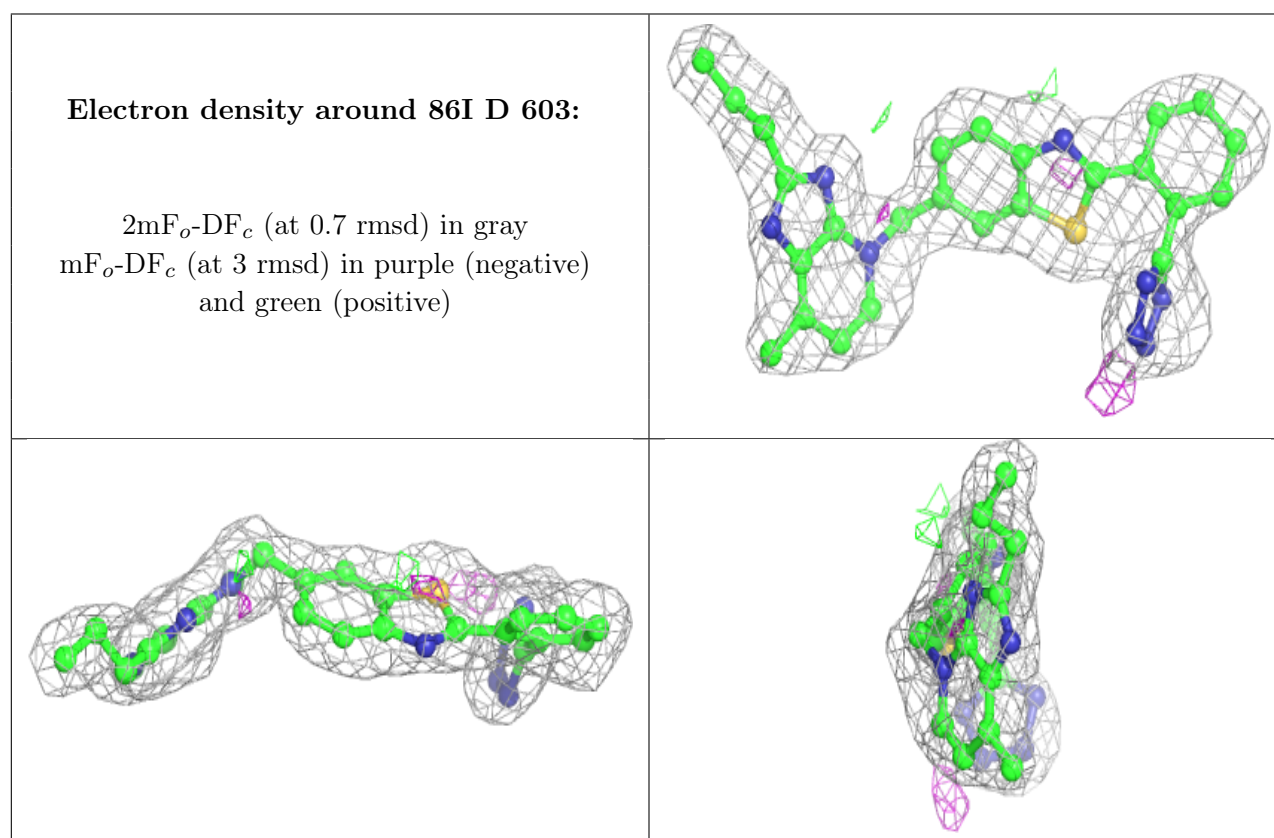
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	86I	D	603	34/34	0.87	0.13	26,37,46,48	0
4	86I	A	603	34/34	0.88	0.14	31,35,42,44	0

*Continued on next page...*

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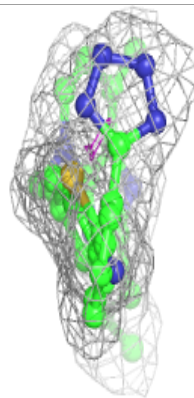
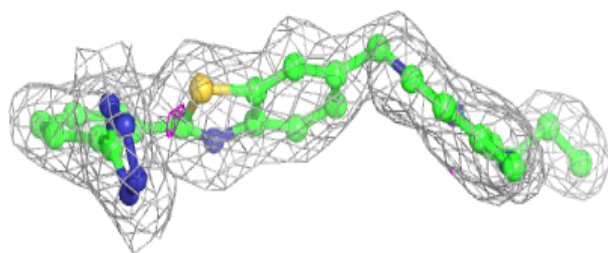
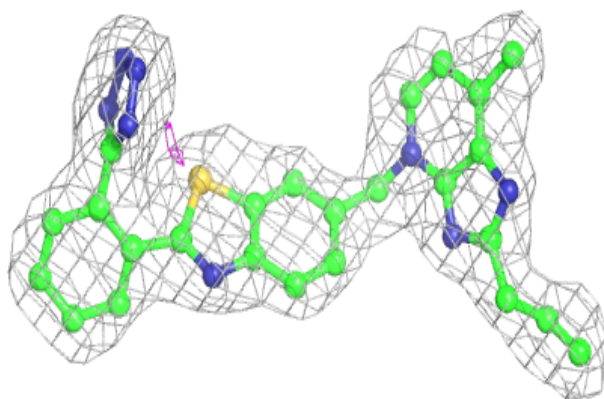
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	86I	B	603	34/34	0.89	0.12	26,33,42,44	0
4	86I	C	603	34/34	0.92	0.11	26,32,39,42	0
3	NDP	D	602	48/48	0.94	0.11	28,36,43,46	0
3	NDP	C	602	48/48	0.95	0.10	30,35,39,42	0
3	NDP	A	602	48/48	0.96	0.12	27,31,35,38	0
3	NDP	B	602	48/48	0.96	0.10	25,29,32,34	0
2	MN	C	601	1/1	0.97	0.09	35,35,35,35	0
2	MN	B	601	1/1	0.98	0.06	38,38,38,38	0
2	MN	A	601	1/1	0.99	0.07	37,37,37,37	0
2	MN	D	601	1/1	0.99	0.07	34,34,34,34	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.

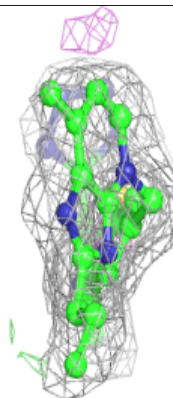
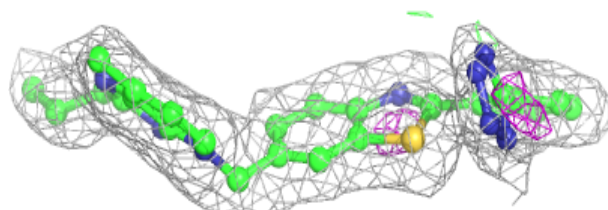
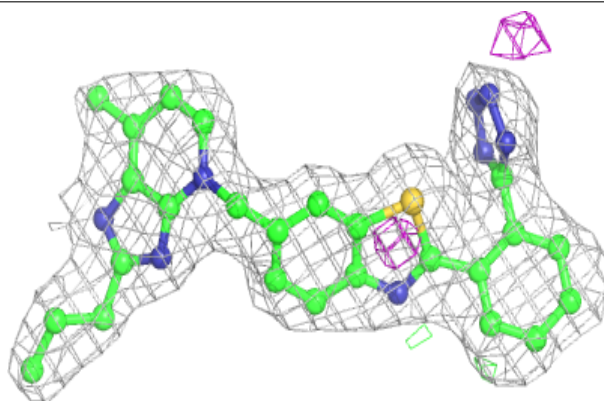


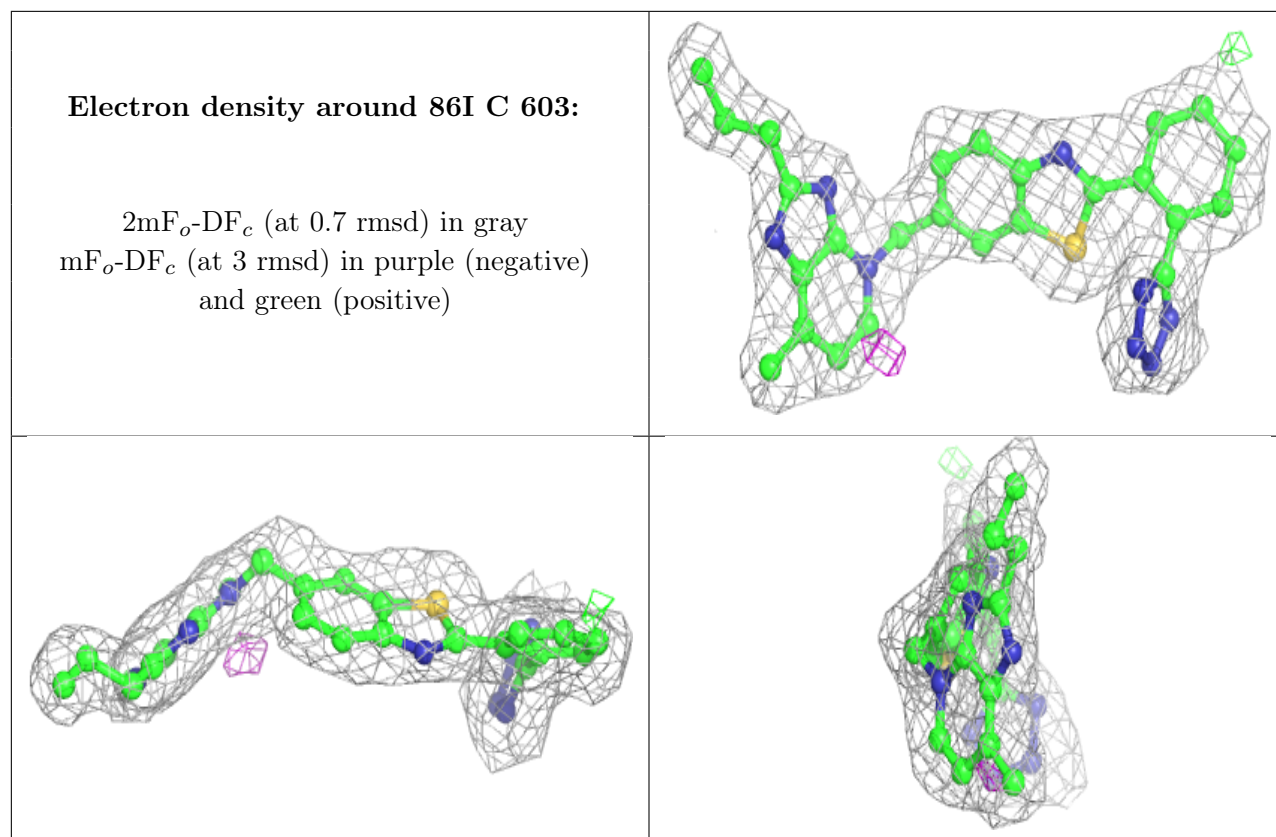
**Electron density around 86I A 603:**

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

**Electron density around 86I B 603:**

$2mF_o-DF_c$  (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.