Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 11:40 AM EST

PDB ID	:	1MBZ
Title	:	BETA-LACTAM SYNTHETASE WITH TRAPPED INTERMEDIATE
Authors	:	Miller, M.T.; Bachmann, B.O.; Townsend, C.A.; Rosenzweig, A.C.
Deposited on	:	2002-08-04
Resolution	:	2.47 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 (i) symbol.

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

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

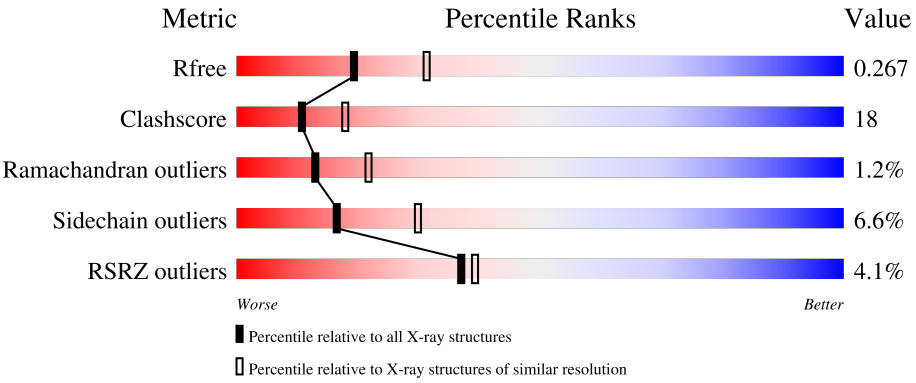
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	513	4% 64% 28%
1	B	513	4% 64% 28%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7918 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.

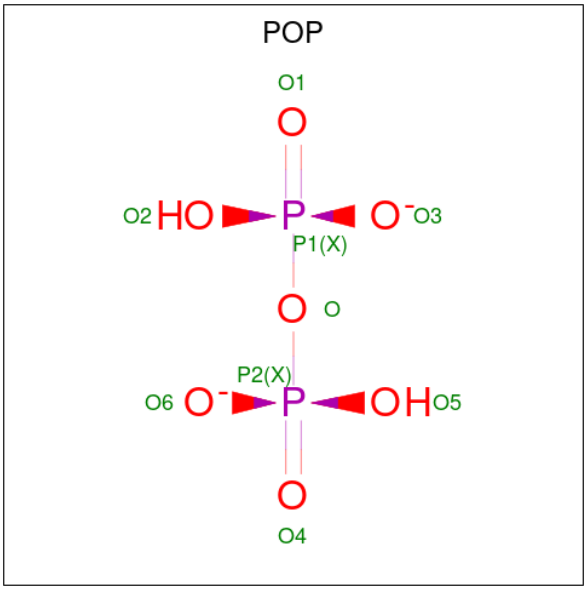
- Molecule 1 is a protein called BETA-LACTAM SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3726	2325	685	708	8			
1	B	494	Total	C	N	O	S	0	0	0
			3717	2319	685	705	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

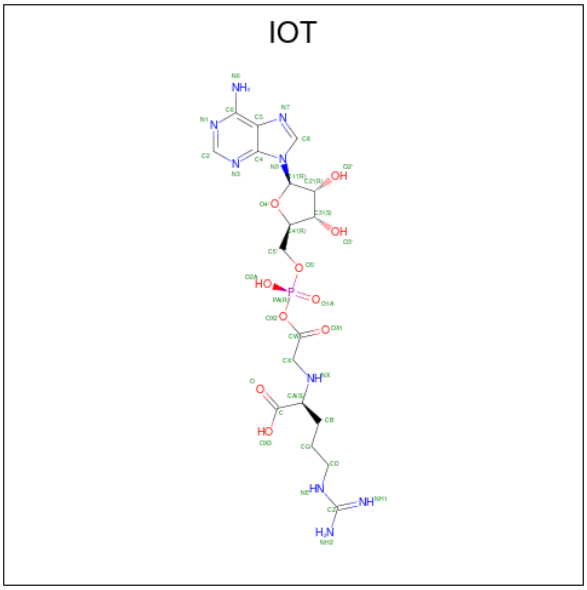
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



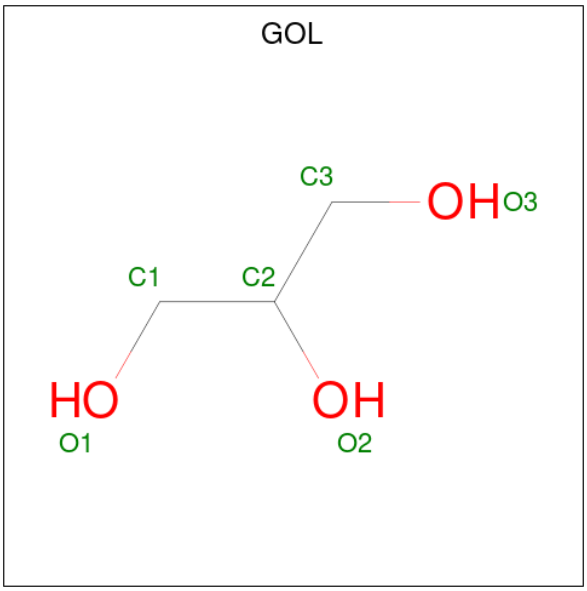
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0

- Molecule 4 is ARGININE-N-METHYLCARBONYL PHOSPHORIC ACID 5'-ADENOSINE ESTER (three-letter code: IOT) (formula: $C_{18}H_{28}N_9O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 38 18 9 10 1	0	0
4	B	1	Total C N O P 38 18 9 10 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

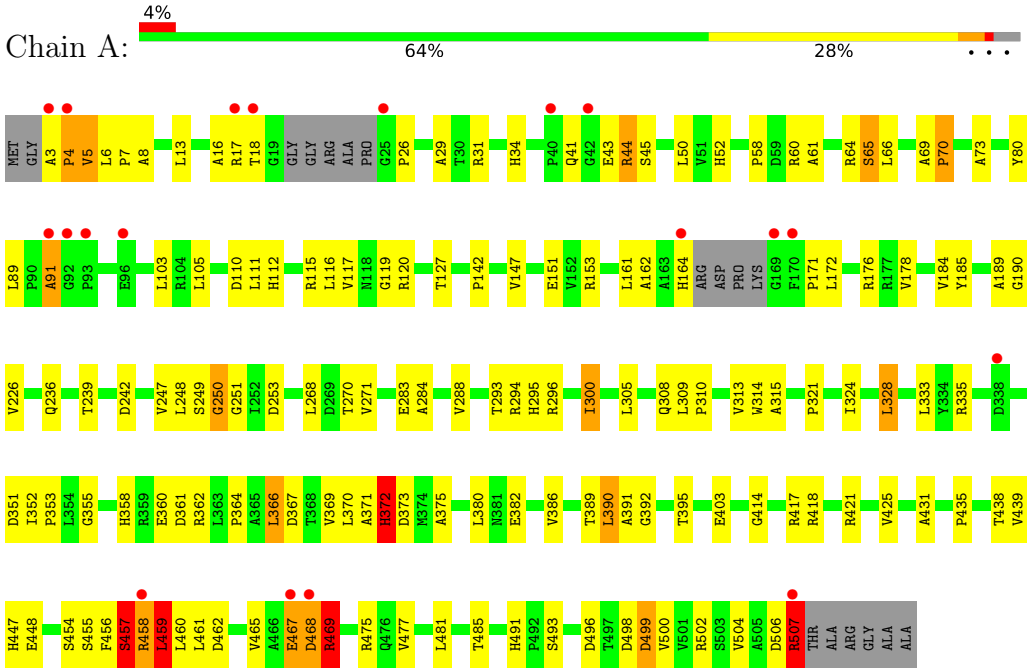
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	203	Total O 203 203	0	0
6	B	162	Total O 162 162	0	0

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.

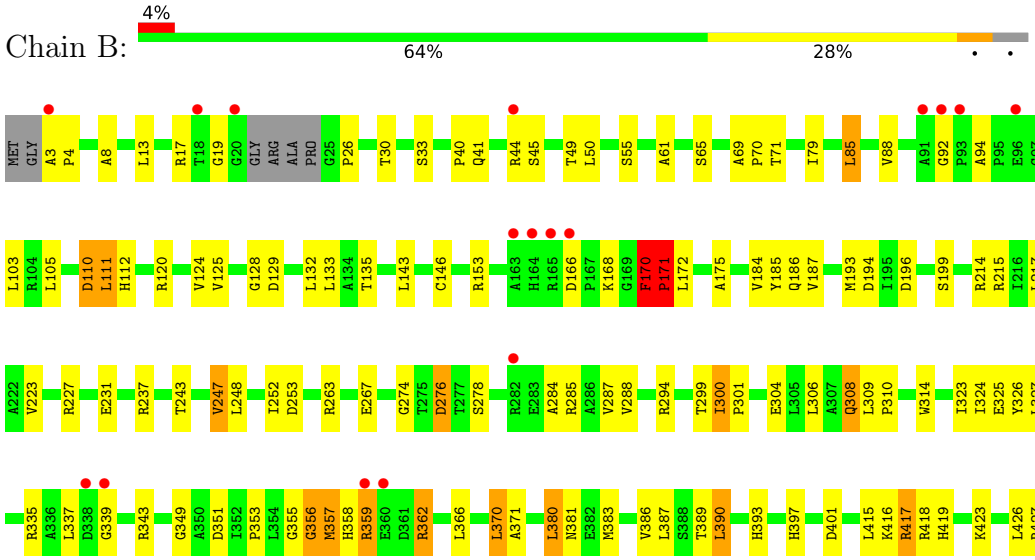
• Molecule 1: BETA-LACTAM SYNTHETASE

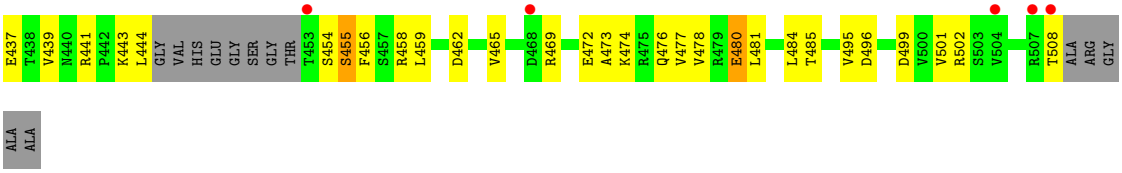
Chain A:



• Molecule 1: BETA-LACTAM SYNTHETASE

Chain B:




E437
T438
V439
N440
R441
P442
K443
L444
GLY
VAL
HIS
GLU
GLY
SER
GLY
THR
T453
S454
S455
F456
S457
R458
L459
D462
V465
D468
R469
E472
A473
K474
R475
Q476
V477
V478
R479
E480
L481
L484
T485
V495
D496
D499
V500
V501
R502
S503
V504
R507
T508
ALA
ARG
GLY
ALA
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.39Å 97.15Å 81.09Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.27 – 2.47 29.27 – 2.46	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.27-2.47) 95.1 (29.27-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.270 0.211 , 0.267	Depositor DCC
R_{free} test set	3030 reflections (8.75%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7918	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: MG, IOT, GOL, POP

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	1.30	3/3800 (0.1%)	0.97	18/5185 (0.3%)
1	B	0.46	0/3791	0.73	4/5172 (0.1%)
All	All	0.98	3/7591 (0.0%)	0.86	22/10357 (0.2%)

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	A	0	6
1	B	0	2
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	ARG	N-CA	68.74	2.83	1.46
1	A	250	GLY	C-N	20.73	1.70	1.33
1	A	459	LEU	C-N	-17.43	0.94	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	SER	C-N-CA	-24.59	60.23	121.70
1	A	250	GLY	O-C-N	-19.38	90.26	123.20
1	A	507	ARG	NE-CZ-NH2	-14.13	113.23	120.30
1	B	170	PHE	CB-CG-CD1	-13.26	111.52	120.80
1	A	69	ALA	C-N-CD	11.26	152.05	128.40
1	B	170	PHE	C-N-CD	10.10	149.60	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	459	LEU	O-C-N	-9.15	108.06	122.70
1	A	507	ARG	NE-CZ-NH1	-9.13	115.73	120.30
1	A	457	SER	CA-C-N	-8.88	97.67	117.20
1	A	469	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	373	ASP	CB-CG-OD2	8.30	125.77	118.30
1	B	171	PRO	CA-N-CD	-8.15	100.09	111.50
1	A	507	ARG	NH1-CZ-NH2	-8.14	110.44	119.40
1	A	468	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	70	PRO	CA-N-CD	-7.15	101.49	111.50
1	B	170	PHE	CG-CD1-CE1	-5.42	114.84	120.80
1	A	457	SER	O-C-N	5.39	131.32	122.70
1	A	250	GLY	C-N-CA	5.38	133.59	122.30
1	A	164	HIS	CA-C-O	5.30	131.22	120.10
1	A	457	SER	N-CA-C	-5.26	96.80	111.00
1	A	372	HIS	CA-CB-CG	5.19	122.43	113.60
1	A	162	ALA	CB-CA-C	5.01	117.61	110.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	457	SER	Mainchain
1	A	459	LEU	Mainchain
1	A	469	ARG	Mainchain,Sidechain
1	A	507	ARG	Sidechain
1	A	70	PRO	Mainchain
1	B	110	ASP	Mainchain
1	B	170	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3726	0	3709	140	0
1	B	3717	0	3704	130	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	0	1	0
3	B	9	0	0	3	0
4	A	38	0	20	4	0
4	B	38	0	21	5	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	203	0	0	15	0
6	B	162	0	0	10	0
All	All	7918	0	7470	275	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 18.

All (275) 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)
4:B:603:IOT:CX	4:B:603:IOT:NX	1.72	1.50
4:A:606:IOT:NX	4:A:606:IOT:CX	1.71	1.49
1:A:250:GLY:C	1:A:251:GLY:N	1.70	1.45
1:A:457:SER:O	1:A:458:ARG:CA	1.99	1.09
1:B:469:ARG:HD2	1:B:508:THR:HG23	1.41	1.02
1:A:455:SER:C	1:A:458:ARG:H	1.64	0.99
1:A:455:SER:O	1:A:458:ARG:N	2.05	0.90
4:A:606:IOT:NX	4:A:606:IOT:CW	2.35	0.88
1:A:456:PHE:C	1:A:458:ARG:N	2.26	0.84
1:A:457:SER:C	1:A:458:ARG:CA	2.46	0.84
1:B:370:LEU:HD23	1:B:371:ALA:N	1.93	0.83
1:A:250:GLY:O	1:A:251:GLY:N	2.10	0.83
1:B:41:GLN:HG2	1:B:45:SER:HB3	1.60	0.82
4:B:603:IOT:NX	4:B:603:IOT:CW	2.39	0.81
1:A:3:ALA:HB3	1:A:242:ASP:OD2	1.80	0.81
1:B:172:LEU:HD13	1:B:193:MET:CE	2.18	0.74
1:A:6:LEU:HB3	1:A:7:PRO:HD2	1.70	0.73
1:A:41:GLN:HG2	1:A:45:SER:HB2	1.72	0.70
1:A:321:PRO:HG3	1:A:475:ARG:HA	1.73	0.70
1:A:17:ARG:HH12	1:A:153:ARG:HD3	1.57	0.69
1:B:443:LYS:HG2	1:B:444:LEU:H	1.59	0.68
1:A:502:ARG:HD3	6:A:760:HOH:O	1.95	0.67
1:B:172:LEU:HD13	1:B:193:MET:HE1	1.74	0.67
1:A:308:GLN:HE21	1:A:335:ARG:HH11	1.41	0.67
1:A:455:SER:C	1:A:458:ARG:N	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HB2	1:B:175:ALA:HB3	1.78	0.66
1:A:3:ALA:N	1:A:342:ARG:HE	1.95	0.65
1:A:13:LEU:HD23	1:A:26:PRO:HB3	1.78	0.65
1:B:359:ARG:HB3	1:B:359:ARG:HH11	1.60	0.65
1:A:382:GLU:HG2	6:A:634:HOH:O	1.97	0.65
1:A:3:ALA:N	1:A:343:ARG:H	1.95	0.64
1:B:310:PRO:HB3	1:B:481:LEU:HD22	1.80	0.64
1:A:3:ALA:HB1	1:A:242:ASP:HB2	1.79	0.63
1:A:457:SER:O	1:A:458:ARG:C	2.36	0.62
1:B:423:LYS:O	1:B:427:ARG:HG3	1.98	0.62
1:A:52:HIS:NE2	1:A:58:PRO:HG3	2.14	0.62
1:A:283:GLU:HG2	1:A:441:ARG:CZ	2.30	0.62
1:A:456:PHE:C	1:A:458:ARG:H	2.01	0.61
1:A:112:HIS:HD2	1:A:115:ARG:HE	1.49	0.61
1:A:176:ARG:HG2	6:A:648:HOH:O	2.00	0.60
1:B:128:GLY:HA2	6:B:733:HOH:O	2.01	0.60
1:B:85:LEU:HG	1:B:105:LEU:HD11	1.83	0.60
1:A:268:LEU:O	1:A:293:THR:HB	2.01	0.60
1:B:217:LEU:HD11	6:B:690:HOH:O	2.01	0.60
1:B:441:ARG:HH11	1:B:441:ARG:HG3	1.65	0.60
1:B:17:ARG:HG2	1:B:19:GLY:H	1.67	0.60
1:A:460:LEU:HD22	1:A:465:VAL:HG11	1.82	0.60
1:B:132:LEU:HD23	1:B:194:ASP:HA	1.82	0.60
1:B:146:CYS:HB3	1:B:168:LYS:O	2.01	0.60
1:B:65:SER:HB3	1:B:71:THR:HB	1.83	0.60
1:A:248:LEU:CD2	1:A:270:THR:HB	2.32	0.60
1:B:170:PHE:O	1:B:171:PRO:O	2.20	0.59
1:A:421:ARG:HE	1:A:440:ASN:HB3	1.66	0.59
1:B:217:LEU:O	6:B:681:HOH:O	2.15	0.59
1:B:459:LEU:CD1	1:B:501:VAL:HG11	2.33	0.59
1:A:13:LEU:CD2	1:A:26:PRO:HB3	2.33	0.59
1:A:73:ALA:HB2	1:A:103:LEU:HD13	1.84	0.58
1:A:283:GLU:HG2	1:A:441:ARG:NE	2.19	0.58
1:B:30:THR:HG23	1:B:389:THR:HB	1.84	0.58
1:B:383:MET:HB3	1:B:397:HIS:CD2	2.38	0.58
1:A:44:ARG:HH21	1:A:44:ARG:HG3	1.67	0.58
1:A:362:ARG:HA	6:A:697:HOH:O	2.04	0.58
1:A:477:VAL:O	1:A:481:LEU:HG	2.04	0.58
1:A:29:ALA:HA	1:A:314:TRP:CH2	2.39	0.58
1:A:17:ARG:HG2	1:A:17:ARG:HH21	1.68	0.57
1:A:248:LEU:HD21	1:A:270:THR:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD23	1:A:391:ALA:N	2.19	0.57
1:B:465:VAL:HG13	1:B:508:THR:HG21	1.87	0.57
1:A:178:VAL:HG23	1:A:184:VAL:O	2.03	0.57
1:B:418:ARG:HG2	1:B:419:HIS:CD2	2.40	0.57
1:A:91:ALA:HB2	6:A:728:HOH:O	2.04	0.57
1:B:252:ILE:HD13	1:B:439:VAL:HA	1.86	0.57
1:A:366:LEU:HD22	1:A:370:LEU:HD23	1.87	0.57
1:B:170:PHE:O	1:B:171:PRO:C	2.41	0.56
1:B:351:ASP:HB2	4:B:603:IOT:OX3	2.05	0.56
1:A:352:ILE:HB	1:A:353:PRO:HD3	1.87	0.56
1:B:349:GLY:O	1:B:353:PRO:HD2	2.05	0.56
1:A:457:SER:O	1:A:458:ARG:HA	1.97	0.56
1:A:31:ARG:HH11	1:A:392:GLY:HA3	1.70	0.56
1:B:3:ALA:HB3	1:B:4:PRO:HD3	1.87	0.55
1:A:85:LEU:HD11	1:A:117:VAL:HG22	1.88	0.55
1:B:111:LEU:HD12	1:B:112:HIS:N	2.21	0.55
1:A:458:ARG:O	1:A:462:ASP:N	2.29	0.55
1:B:218:PRO:HG2	1:B:221:GLU:HB3	1.87	0.55
1:B:219:GLU:O	1:B:223:VAL:HG23	2.07	0.55
1:A:314:TRP:CD1	1:A:485:THR:HB	2.41	0.54
1:A:507:ARG:CZ	1:A:507:ARG:HB3	2.37	0.54
1:A:120:ARG:NE	1:A:395:THR:O	2.36	0.54
1:B:41:GLN:CG	1:B:45:SER:HB3	2.36	0.54
1:A:456:PHE:N	1:A:458:ARG:H	2.05	0.54
1:B:335:ARG:HD3	1:B:390:LEU:HD11	1.89	0.54
1:A:315:ALA:HB1	1:A:386:VAL:HG12	1.89	0.54
4:A:606:IOT:CX	4:A:606:IOT:CA	2.79	0.54
1:B:370:LEU:HD11	1:B:416:LYS:NZ	2.22	0.54
1:B:472:GLU:O	1:B:476:GLN:HG3	2.08	0.54
1:A:116:LEU:HD23	1:B:214:ARG:HB2	1.90	0.54
1:A:226:VAL:HG21	1:A:425:VAL:HG22	1.89	0.54
1:A:491:HIS:CD2	1:A:493:SER:H	2.26	0.54
1:A:352:ILE:HG12	4:A:606:IOT:HE	1.72	0.53
1:B:231:GLU:CD	1:B:263:ARG:HE	2.11	0.53
1:B:274:GLY:O	1:B:299:THR:HA	2.07	0.53
1:B:323:ILE:HG13	1:B:380:LEU:HG	1.89	0.53
1:B:8:ALA:CB	1:B:61:ALA:HB2	2.38	0.53
1:A:372:HIS:O	1:A:375:ALA:N	2.41	0.53
1:A:3:ALA:HB1	1:A:4:PRO:HD2	1.90	0.53
1:B:41:GLN:HG2	1:B:45:SER:CB	2.36	0.53
1:A:496:ASP:HB3	1:A:499:ASP:CG	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PRO:HG2	1:A:438:THR:OG1	2.08	0.53
1:B:366:LEU:HD12	1:B:417:ARG:HB2	1.90	0.53
1:B:436:ALA:HA	1:B:439:VAL:HG22	1.91	0.52
1:A:321:PRO:CG	1:A:475:ARG:HA	2.39	0.52
1:B:26:PRO:HG3	1:B:49:THR:HG21	1.91	0.52
1:A:491:HIS:HD2	1:A:493:SER:H	1.55	0.52
1:B:248:LEU:HD21	1:B:287:VAL:HB	1.91	0.52
1:B:370:LEU:HD11	1:B:416:LYS:HZ3	1.74	0.52
1:A:5:VAL:HB	1:A:239:THR:HG21	1.92	0.52
1:A:34:HIS:HA	1:A:50:LEU:O	2.09	0.52
1:B:351:ASP:OD2	1:B:443:LYS:HD2	2.08	0.52
1:B:125:VAL:HG13	1:B:132:LEU:HB2	1.91	0.52
1:B:386:VAL:HA	1:B:389:THR:OG1	2.09	0.52
1:A:386:VAL:HA	1:A:389:THR:OG1	2.10	0.51
1:B:172:LEU:HD13	1:B:193:MET:HE3	1.88	0.51
1:B:351:ASP:OD2	1:B:356:GLY:HA2	2.10	0.51
1:B:431:ALA:HA	1:B:439:VAL:HG11	1.93	0.51
1:A:358:HIS:CG	1:A:369:VAL:HG11	2.44	0.51
1:B:124:VAL:HG22	1:B:133:LEU:CD2	2.41	0.51
1:B:443:LYS:HG3	3:B:604:POP:P2	2.51	0.51
1:A:313:VAL:HG12	1:A:324:ILE:HD12	1.93	0.51
1:A:467:GLU:C	1:A:469:ARG:H	2.13	0.51
1:B:314:TRP:CD1	1:B:485:THR:HB	2.45	0.51
1:A:300:ILE:HD13	1:A:305:LEU:HD23	1.93	0.51
1:A:380:LEU:HB2	6:A:634:HOH:O	2.10	0.51
1:B:443:LYS:NZ	3:B:604:POP:O4	2.37	0.51
1:A:461:LEU:HD23	1:A:465:VAL:O	2.11	0.51
1:B:327:LEU:HD22	1:B:387:LEU:HD13	1.92	0.51
1:A:8:ALA:HB2	1:A:60:ARG:HB2	1.93	0.50
1:B:13:LEU:HD12	1:B:26:PRO:HB3	1.94	0.50
1:A:17:ARG:HD3	1:A:151:GLU:OE1	2.11	0.50
1:A:44:ARG:HG3	1:A:44:ARG:NH2	2.27	0.50
1:A:43:GLU:HG3	1:A:44:ARG:N	2.25	0.50
1:A:85:LEU:HD13	1:A:105:LEU:HD11	1.94	0.50
1:B:443:LYS:HG2	1:B:444:LEU:N	2.27	0.50
1:A:364:PRO:HB2	6:A:614:HOH:O	2.12	0.50
1:B:308:GLN:OE1	1:B:335:ARG:NH2	2.45	0.50
1:B:358:HIS:NE2	1:B:362:ARG:NH2	2.59	0.50
1:A:3:ALA:CB	1:A:242:ASP:HB2	2.42	0.49
1:A:444:LEU:HD22	1:A:448:GLU:HB2	1.93	0.49
1:B:215:ARG:HG2	6:B:690:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ALA:HA	1:A:439:VAL:HG21	1.94	0.49
1:A:5:VAL:CB	1:A:239:THR:HG21	2.42	0.49
1:A:305:LEU:HD13	1:A:328:LEU:HD13	1.94	0.49
1:B:327:LEU:HD22	1:B:387:LEU:CD1	2.42	0.49
1:A:284:ALA:O	1:A:288:VAL:HG13	2.13	0.49
1:B:474:LYS:O	1:B:478:VAL:HG23	2.12	0.49
1:B:120:ARG:HH21	1:B:120:ARG:HG3	1.78	0.49
1:A:226:VAL:HG21	1:A:425:VAL:CG2	2.43	0.49
1:B:323:ILE:O	1:B:327:LEU:HG	2.13	0.49
4:B:603:IOT:CX	4:B:603:IOT:CA	2.81	0.49
1:B:437:GLU:HG2	1:B:441:ARG:NH2	2.27	0.48
1:A:469:ARG:NH1	1:A:469:ARG:HG3	2.29	0.48
1:A:110:ASP:CG	1:A:111:LEU:H	2.17	0.48
1:B:459:LEU:HD11	1:B:501:VAL:HG11	1.95	0.48
1:B:8:ALA:HB1	1:B:61:ALA:HB2	1.96	0.48
1:A:193:MET:HG2	1:A:204:THR:OG1	2.14	0.47
1:A:65:SER:OG	1:A:66:LEU:N	2.47	0.47
1:A:294:ARG:HD3	6:A:690:HOH:O	2.14	0.47
1:B:69:ALA:O	1:B:71:THR:N	2.42	0.47
1:B:358:HIS:HE1	1:B:362:ARG:O	1.98	0.47
1:A:147:VAL:HB	1:A:172:LEU:HD21	1.97	0.47
1:B:454:SER:O	1:B:458:ARG:HB2	2.15	0.47
1:B:44:ARG:HD3	6:B:763:HOH:O	2.14	0.46
1:B:227:ARG:O	1:B:231:GLU:HB2	2.15	0.46
1:B:247:VAL:HB	4:B:603:IOT:N3	2.29	0.46
1:A:85:LEU:O	1:A:88:VAL:HG22	2.15	0.46
1:A:171:PRO:HA	1:A:185:TYR:OH	2.15	0.46
1:B:496:ASP:OD2	1:B:499:ASP:HB2	2.16	0.46
1:B:418:ARG:HG2	1:B:419:HIS:CG	2.50	0.46
1:A:305:LEU:CD1	1:A:328:LEU:HD13	2.45	0.46
1:B:337:LEU:HD12	1:B:393:HIS:CD2	2.51	0.46
1:A:253:ASP:HB2	3:A:605:POP:O2	2.16	0.46
1:A:3:ALA:HB1	1:A:4:PRO:CD	2.47	0.45
1:A:52:HIS:CD2	1:A:58:PRO:HG3	2.51	0.45
1:A:242:ASP:HA	6:A:660:HOH:O	2.16	0.45
1:A:300:ILE:HD11	1:A:305:LEU:HA	1.98	0.45
1:B:300:ILE:HD11	1:B:304:GLU:C	2.37	0.45
1:B:30:THR:HG23	1:B:389:THR:CB	2.46	0.45
1:A:355:GLY:HA2	6:A:629:HOH:O	2.16	0.45
1:B:326:TYR:O	1:B:330:LEU:HD13	2.16	0.45
1:A:43:GLU:HG3	1:A:44:ARG:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HG23	1:A:247:VAL:O	2.17	0.45
1:A:310:PRO:HA	1:A:313:VAL:HG22	1.98	0.45
1:B:328:LEU:O	1:B:331:THR:HG22	2.17	0.45
1:B:243:THR:OG1	1:B:267:GLU:OE1	2.29	0.45
1:B:351:ASP:HB3	1:B:356:GLY:HA3	1.98	0.45
1:B:129:ASP:HB3	6:B:757:HOH:O	2.16	0.45
1:B:328:LEU:CB	1:B:329:PRO:HD3	2.46	0.45
1:A:344:ILE:HB	1:A:395:THR:HG22	1.99	0.44
1:A:360:GLU:OE2	1:A:362:ARG:NH1	2.49	0.44
1:B:110:ASP:O	1:B:112:HIS:N	2.50	0.44
1:B:132:LEU:HA	1:B:193:MET:O	2.17	0.44
1:B:171:PRO:HD3	1:B:185:TYR:OH	2.17	0.44
1:A:313:VAL:HG21	1:A:481:LEU:HB3	1.99	0.44
1:A:454:SER:O	1:A:458:ARG:N	2.50	0.44
1:B:79:ILE:HD12	1:B:98:ASP:HB3	1.99	0.44
1:B:253:ASP:HB2	3:B:604:POP:O2	2.18	0.44
1:A:308:GLN:HE21	1:A:335:ARG:HD3	1.81	0.44
1:B:124:VAL:HG22	1:B:133:LEU:HD22	1.98	0.44
1:A:447:HIS:H	1:A:447:HIS:CD2	2.34	0.44
1:A:421:ARG:HE	1:A:440:ASN:CB	2.31	0.44
1:A:421:ARG:NE	1:A:440:ASN:HB3	2.32	0.44
1:B:168:LYS:HB2	6:B:756:HOH:O	2.17	0.44
1:A:460:LEU:O	1:A:465:VAL:HG12	2.18	0.44
1:B:110:ASP:C	1:B:112:HIS:N	2.71	0.44
1:B:390:LEU:HD12	1:B:390:LEU:C	2.38	0.44
1:A:308:GLN:NE2	1:A:335:ARG:HD3	2.33	0.44
1:B:323:ILE:HD13	1:B:326:TYR:CD1	2.53	0.43
1:B:324:ILE:HG13	1:B:478:VAL:CG1	2.48	0.43
1:B:92:GLY:O	1:B:94:ALA:N	2.45	0.43
1:B:309:LEU:N	1:B:310:PRO:HD2	2.33	0.43
1:B:328:LEU:HB3	1:B:329:PRO:HD3	1.99	0.43
1:B:359:ARG:HH11	1:B:359:ARG:CB	2.28	0.43
1:A:288:VAL:HG11	1:A:295:HIS:CG	2.54	0.43
1:A:414:GLY:O	1:A:418:ARG:NH1	2.48	0.43
1:A:469:ARG:HG3	1:A:469:ARG:HH11	1.83	0.43
1:B:214:ARG:HG3	6:B:634:HOH:O	2.18	0.43
1:B:325:GLU:HG3	1:B:456:PHE:HD2	1.83	0.43
1:A:333:LEU:HD12	1:A:333:LEU:O	2.19	0.43
1:B:276:ASP:OD1	1:B:301:PRO:HA	2.19	0.43
1:A:491:HIS:HD2	1:A:493:SER:OG	2.02	0.43
1:B:308:GLN:HB3	1:B:328:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:HD2	6:A:766:HOH:O	2.17	0.42
1:B:110:ASP:C	1:B:112:HIS:H	2.22	0.42
1:A:16:ALA:HA	6:A:691:HOH:O	2.18	0.42
1:A:500:VAL:O	1:A:504:VAL:HG23	2.18	0.42
1:B:285:ARG:HG2	1:B:285:ARG:HH21	1.84	0.42
1:B:480:GLU:O	1:B:484:LEU:HG	2.19	0.42
1:B:187:VAL:HG22	1:B:193:MET:SD	2.59	0.42
1:A:80:TYR:CD2	1:A:119:GLY:HA2	2.55	0.42
1:A:247:VAL:HG12	1:A:271:VAL:CG1	2.48	0.42
1:B:495:VAL:HA	6:B:732:HOH:O	2.18	0.42
1:A:189:ALA:O	1:A:190:GLY:C	2.57	0.42
1:B:237:ARG:O	1:B:343:ARG:HD3	2.20	0.42
1:A:371:ALA:HB2	6:A:626:HOH:O	2.19	0.42
1:A:458:ARG:O	1:A:461:LEU:N	2.53	0.42
1:B:458:ARG:O	1:B:462:ASP:N	2.53	0.42
1:A:153:ARG:HG3	1:A:153:ARG:HH11	1.84	0.41
1:B:146:CYS:SG	1:B:184:VAL:HG22	2.60	0.41
1:A:89:LEU:HD21	1:A:105:LEU:HD23	2.02	0.41
1:A:193:MET:HB3	1:A:193:MET:HE2	1.69	0.41
1:A:8:ALA:HB3	1:A:61:ALA:HB2	2.03	0.41
1:A:309:LEU:N	1:A:310:PRO:HD2	2.35	0.41
1:A:444:LEU:HD23	1:A:444:LEU:HA	1.84	0.41
1:B:473:ALA:O	1:B:477:VAL:HG23	2.20	0.41
1:A:73:ALA:CB	1:A:103:LEU:HD13	2.49	0.41
1:A:248:LEU:HD22	1:A:270:THR:HB	2.02	0.41
1:B:79:ILE:HG21	1:B:85:LEU:HD23	2.03	0.41
1:B:306:LEU:HD21	1:B:455:SER:HB2	2.01	0.41
1:A:236:GLN:HE21	1:A:236:GLN:HB2	1.67	0.41
1:B:85:LEU:O	1:B:88:VAL:HG22	2.21	0.41
1:B:103:LEU:HD12	1:B:103:LEU:HA	1.92	0.41
1:A:361:ASP:OD1	1:A:361:ASP:N	2.54	0.41
1:B:308:GLN:CD	1:B:335:ARG:HH21	2.24	0.41
1:B:355:GLY:O	1:B:357:MET:N	2.54	0.41
1:A:127:THR:HG23	1:A:127:THR:O	2.21	0.40
1:A:351:ASP:O	1:A:355:GLY:N	2.53	0.40
1:B:459:LEU:HD13	1:B:459:LEU:C	2.40	0.40
1:B:186:GLN:HE22	1:B:381:ASN:HD21	1.69	0.40
1:B:252:ILE:HG23	1:B:253:ASP:N	2.36	0.40
1:B:284:ALA:O	1:B:288:VAL:HG23	2.20	0.40
1:B:237:ARG:HH11	1:B:237:ARG:HG3	1.86	0.40
1:A:370:LEU:HD21	6:A:613:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ARG:HD2	6:A:714:HOH:O	2.21	0.40
1:B:196:ASP:HB3	1:B:199:SER:OG	2.21	0.40
1:B:454:SER:HB2	6:B:718:HOH:O	2.22	0.40
1:B:324:ILE:HG13	1:B:478:VAL:HG11	2.04	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	490/513 (96%)	453 (92%)	31 (6%)	6 (1%)	13	22
1	B	488/513 (95%)	444 (91%)	38 (8%)	6 (1%)	13	22
All	All	978/1026 (95%)	897 (92%)	69 (7%)	12 (1%)	13	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	LEU
1	B	339	GLY
1	A	459	LEU
1	A	467	GLU
1	A	468	ASP
1	B	356	GLY
1	A	4	PRO
1	A	91	ALA
1	A	5	VAL
1	B	40	PRO
1	B	171	PRO
1	B	70	PRO

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	386/395 (98%)	364 (94%)	22 (6%)	20	37
1	B	385/395 (98%)	356 (92%)	29 (8%)	13	24
All	All	771/790 (98%)	720 (93%)	51 (7%)	16	30

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	44	ARG
1	A	65	SER
1	A	86	LEU
1	A	142	PRO
1	A	161	LEU
1	A	249	SER
1	A	296	ARG
1	A	300	ILE
1	A	328	LEU
1	A	345	LEU
1	A	366	LEU
1	A	367	ASP
1	A	372	HIS
1	A	390	LEU
1	A	403	GLU
1	A	444	LEU
1	A	469	ARG
1	A	498	ASP
1	A	499	ASP
1	A	506	ASP
1	A	507	ARG
1	B	33	SER
1	B	50	LEU
1	B	55	SER
1	B	85	LEU
1	B	101	LEU

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Mol	Chain	Res	Type
1	B	135	THR
1	B	143	LEU
1	B	153	ARG
1	B	166	ASP
1	B	247	VAL
1	B	276	ASP
1	B	278	SER
1	B	294	ARG
1	B	300	ILE
1	B	308	GLN
1	B	328	LEU
1	B	357	MET
1	B	359	ARG
1	B	362	ARG
1	B	370	LEU
1	B	380	LEU
1	B	390	LEU
1	B	401	ASP
1	B	415	LEU
1	B	417	ARG
1	B	426	LEU
1	B	455	SER
1	B	480	GLU
1	B	502	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	118	ASN
1	A	186	GLN
1	A	236	GLN
1	A	308	GLN
1	A	491	HIS
1	B	41	GLN
1	B	290	HIS
1	B	381	ASN
1	B	440	ASN
1	B	471	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	POP	A	605	2	6,8,8	1.11	0	13,13,13	0.83	0
3	POP	B	604	2	6,8,8	1.11	0	13,13,13	0.80	0
5	GOL	B	605	-	5,5,5	0.92	0	5,5,5	0.40	0
4	IOT	B	603	2	36,40,40	4.90	11 (30%)	38,57,57	2.88	14 (36%)
5	GOL	A	607	-	5,5,5	0.85	0	5,5,5	0.38	0
4	IOT	A	606	2	36,40,40	4.60	12 (33%)	38,57,57	3.03	15 (39%)

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	POP	A	605	2	-	0/6/6/6	-
3	POP	B	604	2	-	0/6/6/6	-
5	GOL	B	605	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IOT	B	603	2	-	10/25/47/47	0/3/3/3
5	GOL	A	607	-	-	2/4/4/4	-
4	IOT	A	606	2	-	10/25/47/47	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	IOT	CX-NX	21.67	1.72	1.46
4	A	606	IOT	CX-NX	20.70	1.71	1.46
4	A	606	IOT	CX-CW	-11.76	1.13	1.50
4	B	603	IOT	CX-CW	-11.34	1.14	1.50
4	B	603	IOT	OX1-CW	7.60	1.45	1.22
4	B	603	IOT	C4-N3	7.09	1.45	1.35
4	A	606	IOT	C4-N3	6.69	1.44	1.35
4	B	603	IOT	C2-N1	5.84	1.44	1.33
4	A	606	IOT	C2-N1	5.76	1.44	1.33
4	B	603	IOT	PA-OX2	-5.53	1.49	1.60
4	A	606	IOT	OX1-CW	4.91	1.37	1.22
4	A	606	IOT	PA-O5'	-4.31	1.41	1.59
4	B	603	IOT	PA-O5'	-3.75	1.44	1.59
4	B	603	IOT	C2-N3	3.54	1.37	1.32
4	A	606	IOT	C2'-C1'	-3.50	1.48	1.53
4	B	603	IOT	C2'-C1'	-3.49	1.48	1.53
4	A	606	IOT	C2-N3	3.02	1.37	1.32
4	B	603	IOT	C5'-C4'	-2.86	1.42	1.51
4	A	606	IOT	C6-N6	-2.77	1.23	1.34
4	B	603	IOT	C6-N6	-2.77	1.23	1.34
4	A	606	IOT	O3'-C3'	-2.63	1.36	1.43
4	A	606	IOT	C5'-C4'	-2.38	1.44	1.51
4	A	606	IOT	C6-C5	2.05	1.50	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	606	IOT	O5'-C5'-C4'	8.37	137.81	108.99
4	B	603	IOT	O5'-C5'-C4'	7.81	135.87	108.99
4	A	606	IOT	C3'-C2'-C1'	7.40	112.12	100.98
4	B	603	IOT	C3'-C2'-C1'	6.59	110.91	100.98
4	A	606	IOT	OX2-PA-O5'	-6.44	84.13	102.92
4	B	603	IOT	O5'-PA-O1A	5.96	132.36	109.07
4	A	606	IOT	O5'-PA-O1A	5.64	131.11	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	IOT	N3-C2-N1	-5.31	120.39	128.68
4	A	606	IOT	N3-C2-N1	-5.17	120.60	128.68
4	A	606	IOT	C2-N1-C6	4.71	126.82	118.75
4	B	603	IOT	C2-N1-C6	4.66	126.72	118.75
4	B	603	IOT	OX2-PA-O5'	-4.65	89.34	102.92
4	B	603	IOT	O2A-PA-O5'	-4.48	86.96	107.75
4	B	603	IOT	O2A-PA-OX2	4.31	118.22	104.14
4	A	606	IOT	O2A-PA-O5'	-4.26	87.95	107.75
4	A	606	IOT	OX2-PA-O1A	3.49	120.20	109.45
4	B	603	IOT	CX-NX-CA	3.35	121.03	114.01
4	A	606	IOT	C5-C6-N1	-3.26	112.97	120.35
4	A	606	IOT	O3'-C3'-C4'	3.10	120.00	111.05
4	B	603	IOT	C5-C6-N1	-3.08	113.37	120.35
4	A	606	IOT	CX-NX-CA	3.05	120.41	114.01
4	B	603	IOT	O3'-C3'-C4'	2.86	119.31	111.05
4	B	603	IOT	O4'-C4'-C5'	-2.68	100.55	109.37
4	B	603	IOT	C5-C6-N6	2.64	124.36	120.35
4	A	606	IOT	C5-C6-N6	2.59	124.29	120.35
4	A	606	IOT	O4'-C4'-C5'	-2.45	101.31	109.37
4	A	606	IOT	O4'-C1'-C2'	-2.10	103.85	106.93
4	B	603	IOT	OX1-CW-CX	-2.04	117.00	123.64
4	A	606	IOT	N6-C6-N1	2.01	122.74	118.57

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	IOT	OX2-CW-CX-NX
4	A	606	IOT	NH1-CZ-NE-CD
4	A	606	IOT	NH2-CZ-NE-CD
4	B	603	IOT	NH1-CZ-NE-CD
4	B	603	IOT	NH2-CZ-NE-CD
5	B	605	GOL	C1-C2-C3-O3
4	A	606	IOT	NX-CA-CB-CG
4	A	606	IOT	OX1-CW-CX-NX
4	B	603	IOT	NX-CA-CB-CG
4	A	606	IOT	C-CA-CB-CG
5	A	607	GOL	O1-C1-C2-C3
4	B	603	IOT	C-CA-CB-CG
5	B	605	GOL	O2-C2-C3-O3
4	B	603	IOT	OX1-CW-CX-NX
4	A	606	IOT	NE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
4	A	606	IOT	CB-CA-NX-CX
4	B	603	IOT	CB-CA-NX-CX
4	A	606	IOT	C-CA-NX-CX
4	B	603	IOT	C-CA-NX-CX
4	B	603	IOT	C4'-C5'-O5'-PA
5	A	607	GOL	O1-C1-C2-O2
4	B	603	IOT	C3'-C4'-C5'-O5'
4	B	603	IOT	CW-CX-NX-CA
4	A	606	IOT	CW-OX2-PA-O2A

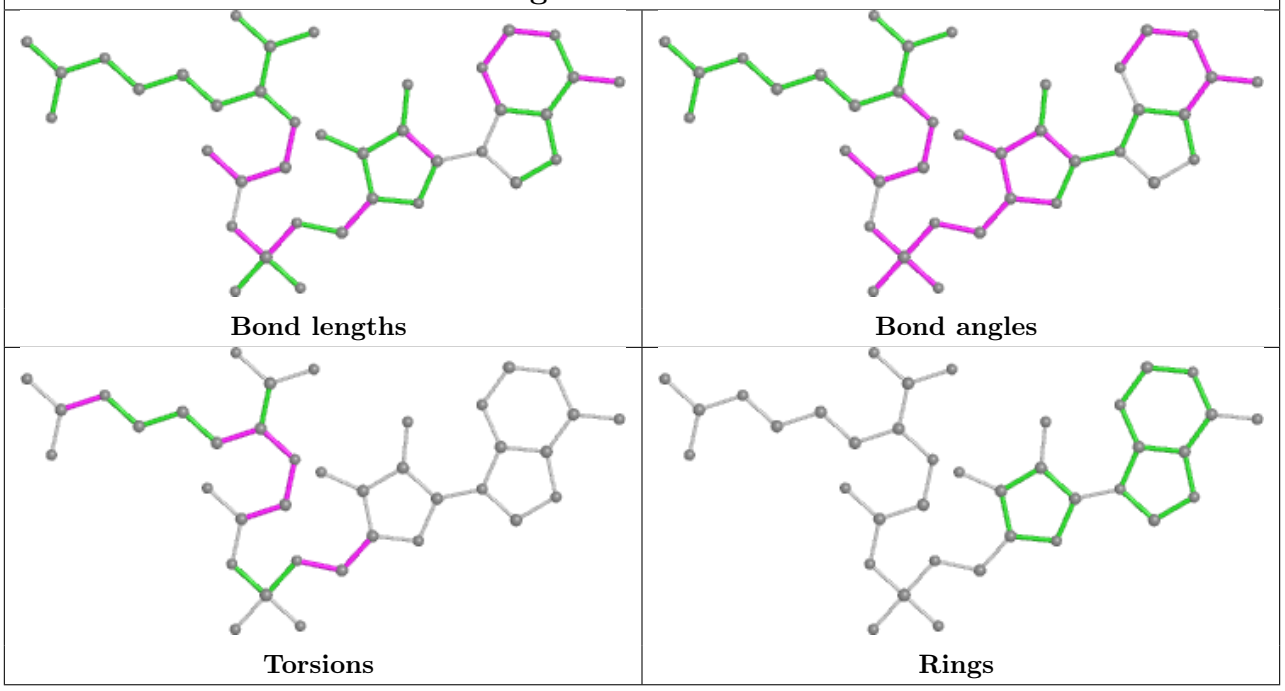
There are no ring outliers.

4 monomers are involved in 13 short contacts:

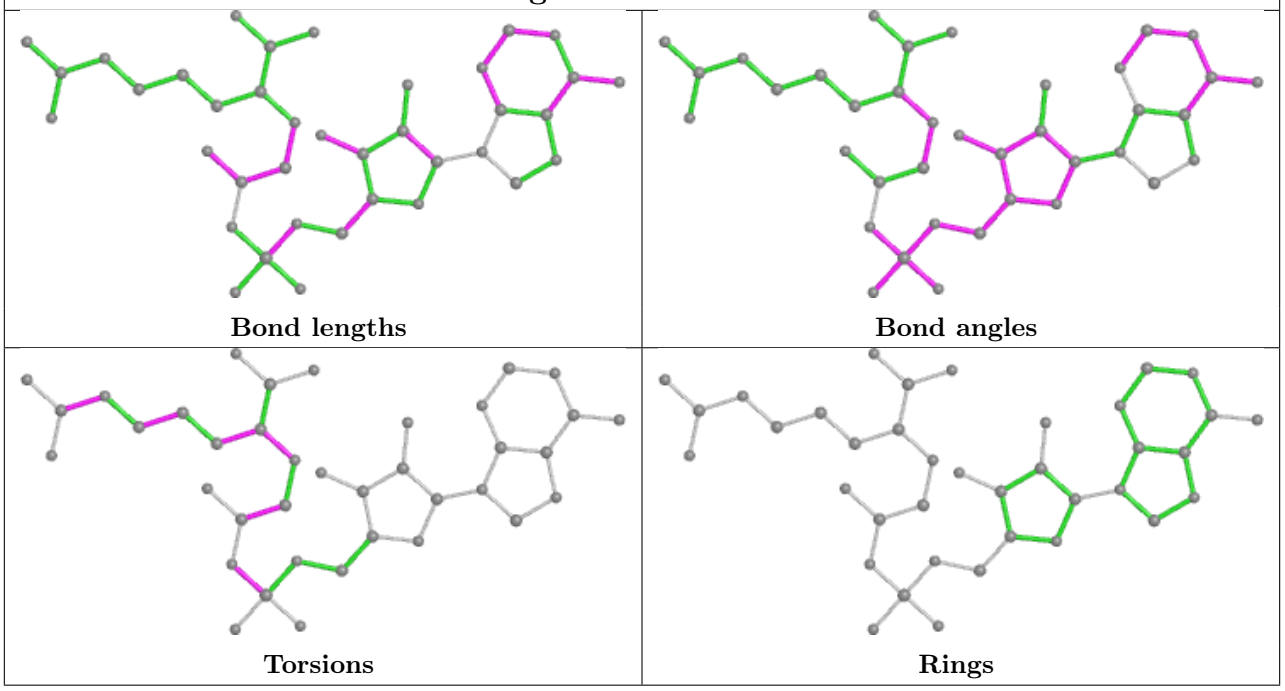
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	POP	1	0
3	B	604	POP	3	0
4	B	603	IOT	5	0
4	A	606	IOT	4	0

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 IOT B 603



Ligand IOT A 606



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	250:GLY	C	251:GLY	N	1.70
1	A	459:LEU	C	460:LEU	N	0.94

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	496/513 (96%)	-0.07	19 (3%)	40	42	2, 16, 42, 59	0
1	B	494/513 (96%)	0.02	22 (4%)	33	35	3, 18, 44, 64	0
All	All	990/1026 (96%)	-0.03	41 (4%)	37	39	2, 17, 44, 64	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ALA	8.4
1	A	3	ALA	6.9
1	A	4	PRO	5.8
1	A	93	PRO	5.3
1	A	507	ARG	5.2
1	B	93	PRO	4.8
1	B	91	ALA	4.7
1	B	92	GLY	4.6
1	A	18	THR	4.5
1	B	164	HIS	4.2
1	B	165	ARG	4.1
1	B	3	ALA	4.0
1	B	166	ASP	3.8
1	A	96	GLU	3.6
1	A	164	HIS	3.5
1	B	359	ARG	3.5
1	B	453	THR	3.5
1	A	92	GLY	3.4
1	A	468	ASP	3.2
1	A	338	ASP	3.0
1	A	467	GLU	3.0
1	A	42	GLY	2.9
1	B	18	THR	2.7
1	B	338	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	504	VAL	2.7
1	B	20	GLY	2.6
1	B	468	ASP	2.5
1	A	17	ARG	2.5
1	B	44	ARG	2.3
1	B	282	ARG	2.3
1	A	170	PHE	2.3
1	A	40	PRO	2.2
1	A	169	GLY	2.2
1	A	458	ARG	2.2
1	B	339	GLY	2.1
1	B	360	GLU	2.1
1	A	25	GLY	2.1
1	B	507	ARG	2.1
1	B	508	THR	2.0
1	B	163	ALA	2.0
1	B	96	GLU	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
5	GOL	B	605	6/6	0.66	0.28	38,39,40,40	0
2	MG	B	602	1/1	0.81	0.14	18,18,18,18	0
5	GOL	A	607	6/6	0.85	0.16	34,34,35,37	0
2	MG	B	601	1/1	0.86	0.06	23,23,23,23	0
2	MG	A	603	1/1	0.86	0.09	10,10,10,10	0
4	IOT	B	603	38/38	0.90	0.17	23,28,35,36	0

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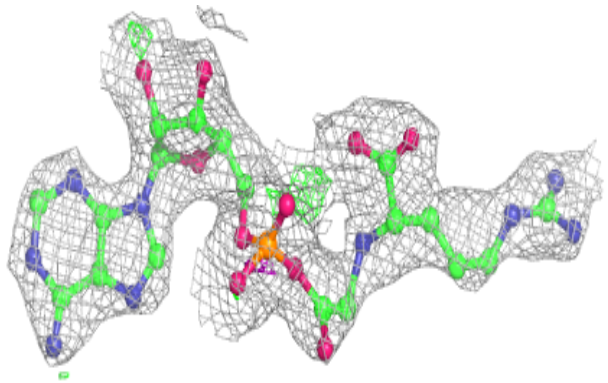
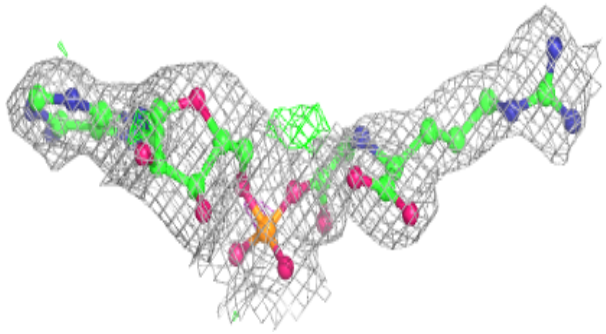
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IOT	A	606	38/38	0.94	0.16	10,16,25,26	0
3	POP	A	605	9/9	0.98	0.11	4,7,16,16	0
3	POP	B	604	9/9	0.98	0.10	18,20,21,22	0
2	MG	A	604	1/1	0.98	0.11	14,14,14,14	0

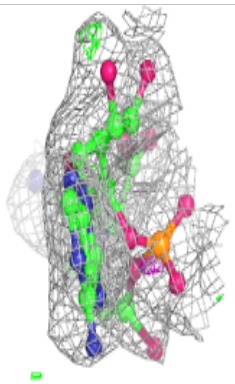
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IOT 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)

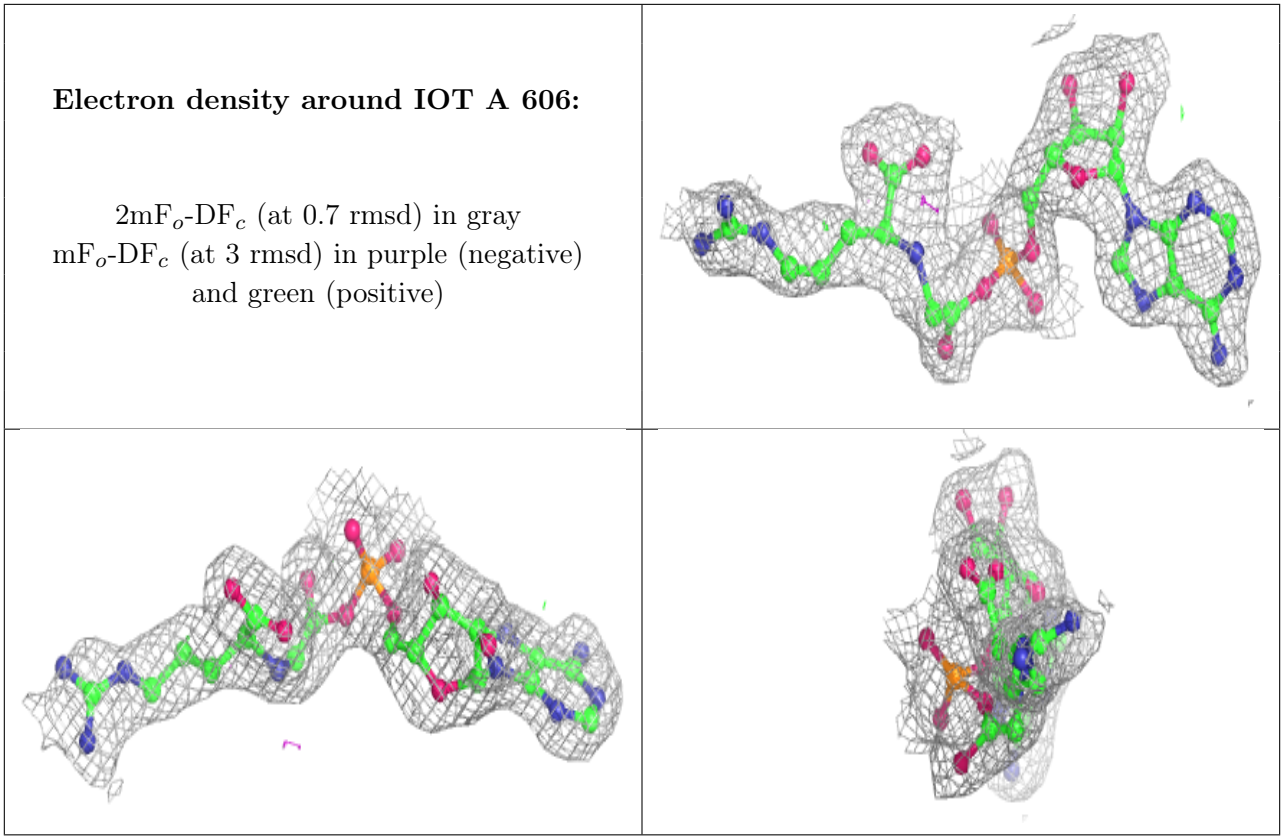






Electron density around IOT A 606:

$2mF_o$-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.