



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2025 – 01:18 pm BST

PDB ID : 9G46 / pdb_00009g46
Title : The structure of Candida albicans phosphoglucose isomerase (CaPGI) in complex with fragments
Authors : Yan, K.
Deposited on : 2024-07-14
Resolution : 1.44 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

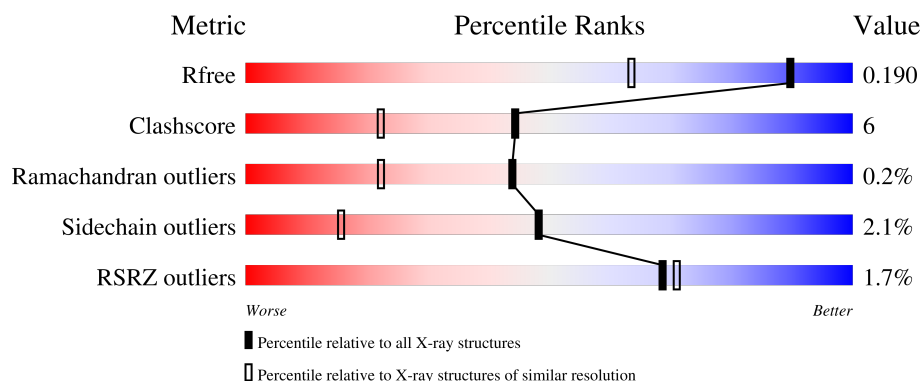
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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}	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	555	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9880 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.

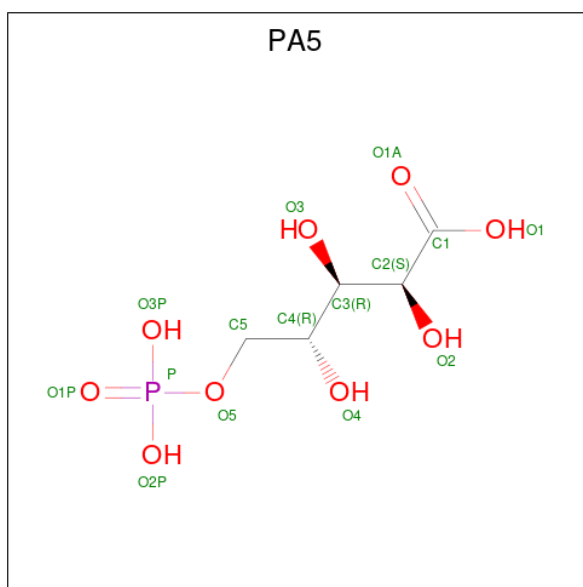
- Molecule 1 is a protein called Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	10	0
			4343	2793	715	823	12			
1	B	550	Total	C	N	O	S	0	12	0
			4355	2800	718	825	12			

There are 10 discrepancies between the modelled and reference sequences:

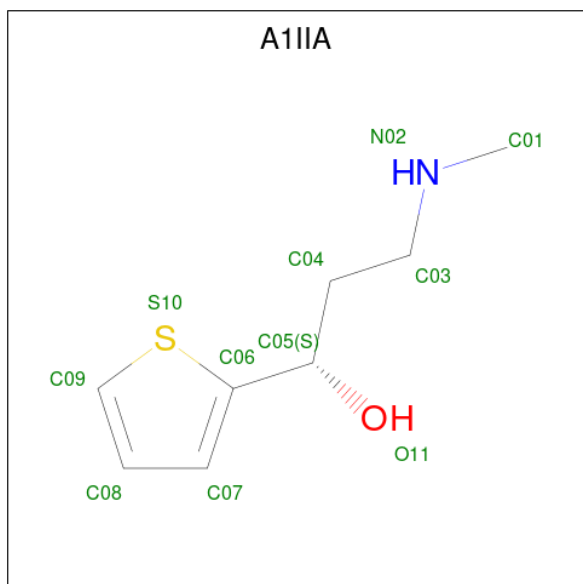
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P83780
A	-3	PRO	-	expression tag	UNP P83780
A	-2	LEU	-	expression tag	UNP P83780
A	-1	GLY	-	expression tag	UNP P83780
A	0	SER	-	expression tag	UNP P83780
B	-4	GLY	-	expression tag	UNP P83780
B	-3	PRO	-	expression tag	UNP P83780
B	-2	LEU	-	expression tag	UNP P83780
B	-1	GLY	-	expression tag	UNP P83780
B	0	SER	-	expression tag	UNP P83780

- Molecule 2 is 5-PHOSPHOARABINONIC ACID (CCD ID: PA5) (formula: C₅H₁₁O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			15	5	9	1		
2	B	1	Total	C	O	P	0	0
			15	5	9	1		

- Molecule 3 is (1S)-3-(methylamino)-1-thiophen-2-yl-propan-1-ol (CCD ID: A1IIA) (formula: C₈H₁₃NOS) (labeled as "Ligand of Interest" by depositor).



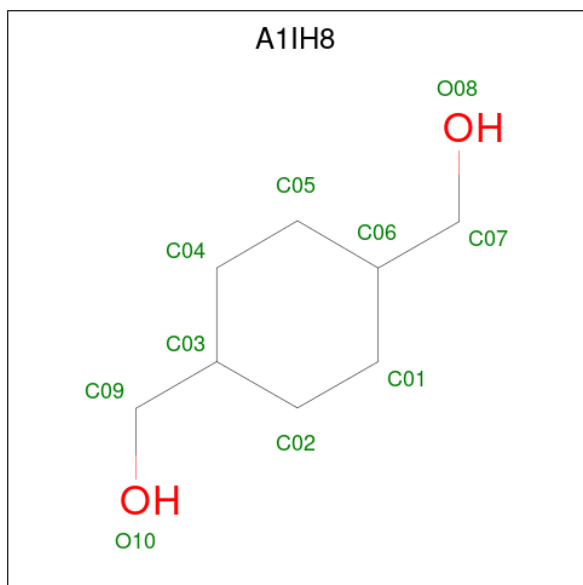
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			11	8	1	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			11	8	1	1	1		

- Molecule 4 is [4-(hydroxymethyl)cyclohexyl]methanol (CCD ID: A1IH8) (formula: C₈H₁₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	8	2		
4	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	564	Total	O	0	0
			564	564		

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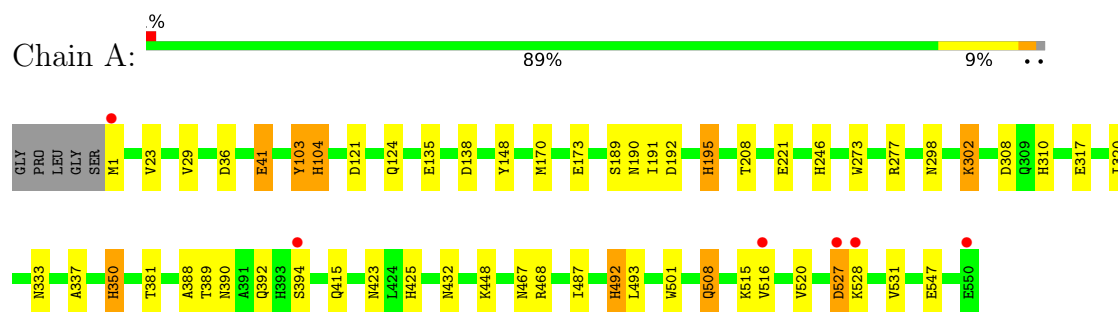
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	544	Total 544	O 544	0	0

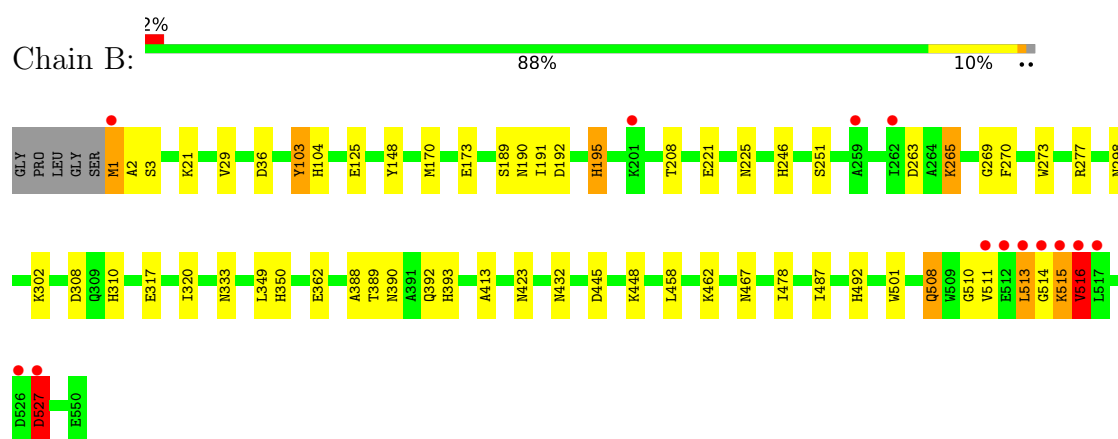
3 Residue-property plots [i](#)

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: Glucose-6-phosphate isomerase



- Molecule 1: Glucose-6-phosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.77Å 101.17Å 133.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 1.44 29.82 – 1.44	Depositor EDS
% Data completeness (in resolution range)	80.4 (29.82-1.44) 80.8 (29.82-1.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.155 , 0.179 0.167 , 0.190	Depositor DCC
R_{free} test set	10605 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9880	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3624e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, A1IH8, PA5, A1IIA

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	0.72	2/4477 (0.0%)	1.04	11/6069 (0.2%)
1	B	0.73	2/4493 (0.0%)	1.05	5/6087 (0.1%)
All	All	0.72	4/8970 (0.0%)	1.05	16/12156 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	GLU	CD-OE2	-5.32	1.15	1.25
1	B	36	ASP	CG-OD2	5.06	1.34	1.25
1	A	36	ASP	CG-OD2	5.04	1.34	1.25
1	A	394	SER	CB-OG	5.01	1.52	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	ASP	CA-CB-CG	8.59	121.19	112.60
1	B	445	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	41	GLU	CB-CG-CD	5.90	122.62	112.60
1	A	350	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	B	527	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	36	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	492	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	121	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	104	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	468	ARG	CB-CA-C	5.12	115.69	109.85
1	B	221	GLU	N-CA-CB	5.11	117.41	110.01
1	A	302	LYS	CG-CD-CE	5.07	122.96	111.30
1	A	492	HIS	CB-CG-ND1	5.05	130.27	122.70
1	B	270	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	510	GLY	O-C-N	-5.03	117.31	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ASP	CA-CB-CG	5.02	117.62	112.60

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	4343	0	4258	50	0
1	B	4355	0	4280	54	0
2	A	15	0	8	1	0
2	B	15	0	8	0	0
3	A	11	0	0	0	0
3	B	11	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	564	0	0	22	1
6	B	544	0	0	10	1
All	All	9880	0	8554	102	1

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 (102) 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:A:381[A]:THR:HG22	6:A:701:HOH:O	1.30	1.21
1:B:317:GLU:CG	6:B:1210:HOH:O	1.96	1.11
1:A:423:ASN:CG	6:A:705:HOH:O	2.00	1.03
1:A:527:ASP:HB3	6:A:1125:HOH:O	1.67	0.94
1:B:310:HIS:HE1	1:B:320:ILE:H	1.18	0.92
1:A:310:HIS:HE1	1:A:320:ILE:H	1.20	0.90
1:B:277:ARG:HH22	1:B:508:GLN:HE21	1.22	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520[A]:VAL:HG23	6:A:794:HOH:O	1.76	0.84
1:B:513:LEU:O	1:B:513:LEU:HD23	1.79	0.83
1:A:381[A]:THR:CG2	6:A:701:HOH:O	1.98	0.79
1:A:277:ARG:HH22	1:A:508:GLN:HE21	1.28	0.79
1:A:124:GLN:NE2	6:A:702:HOH:O	2.16	0.78
1:A:547:GLU:HG3	6:A:1101:HOH:O	1.88	0.74
1:A:415[A]:GLN:NE2	6:A:703:HOH:O	2.23	0.71
1:B:148:TYR:H	1:B:246:HIS:HE1	1.37	0.70
1:B:527:ASP:HB3	6:B:1083:HOH:O	1.92	0.70
1:A:392:GLN:HE22	1:A:432:ASN:HB3	1.56	0.69
1:B:190:ASN:H	1:B:195:HIS:HD2	1.40	0.68
1:B:392:GLN:HE22	1:B:432:ASN:HB3	1.59	0.67
1:A:333:ASN:HD21	1:A:501:TRP:HE1	1.43	0.67
1:A:390:ASN:ND2	6:A:706:HOH:O	2.28	0.66
1:A:190:ASN:H	1:A:195:HIS:HD2	1.44	0.66
1:A:148:TYR:H	1:A:246:HIS:HE1	1.42	0.66
1:A:208:THR:O	1:A:246:HIS:HD2	1.79	0.65
1:B:308:ASP:OD1	1:B:492:HIS:HE1	1.80	0.64
1:A:308:ASP:OD1	1:A:492:HIS:HE1	1.80	0.64
2:A:601:PA5:O4	1:B:393:HIS:HD2	1.81	0.63
1:A:317:GLU:H	1:A:317:GLU:CD	2.04	0.63
1:A:337:ALA:O	6:A:701:HOH:O	2.15	0.63
1:B:173:GLU:OE1	1:B:350:HIS:HE1	1.81	0.63
1:A:390:ASN:CG	6:A:706:HOH:O	2.41	0.63
1:B:513:LEU:HD23	1:B:513:LEU:C	2.24	0.62
1:B:208:THR:O	1:B:246:HIS:HD2	1.83	0.62
1:B:390:ASN:HD22	1:B:390:ASN:H	1.48	0.61
1:A:333:ASN:ND2	1:A:501:TRP:HE1	1.98	0.61
1:A:350:HIS:HD2	6:A:1167:HOH:O	1.83	0.60
1:B:333:ASN:HD21	1:B:501:TRP:HE1	1.50	0.60
1:A:423:ASN:CB	6:A:705:HOH:O	2.44	0.59
1:B:350:HIS:HD2	6:B:1160:HOH:O	1.84	0.59
1:A:173:GLU:OE1	1:A:350:HIS:HE1	1.84	0.59
1:A:221:GLU:OE2	1:B:393:HIS:HE1	1.87	0.58
1:A:310:HIS:CE1	1:A:320:ILE:H	2.11	0.57
1:B:29:VAL:H	1:B:467:ASN:ND2	2.02	0.57
1:B:310:HIS:CE1	1:B:320:ILE:H	2.09	0.57
1:A:423:ASN:HB2	6:A:705:HOH:O	2.03	0.56
1:A:277:ARG:HH22	1:A:508:GLN:NE2	2.02	0.56
1:B:333:ASN:ND2	1:B:501:TRP:HE1	2.04	0.55
1:A:135[B]:GLU:HG3	6:A:949:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ARG:HH22	1:B:508:GLN:NE2	1.99	0.55
1:B:148:TYR:N	1:B:246:HIS:HE1	2.05	0.55
1:A:148:TYR:N	1:A:246:HIS:HE1	2.06	0.53
1:A:310:HIS:HD2	6:A:1199:HOH:O	1.91	0.53
1:B:104:HIS:HD2	6:B:1021:HOH:O	1.92	0.52
1:B:189:SER:H	1:B:195:HIS:CD2	2.27	0.52
1:A:41:GLU:HG2	6:A:1191:HOH:O	2.10	0.52
1:B:125[B]:GLU:OE2	6:B:701:HOH:O	2.19	0.51
1:B:263[A]:ASP:CG	1:B:265:LYS:HG2	2.36	0.51
1:A:104:HIS:HD2	6:A:992:HOH:O	1.92	0.50
1:B:513:LEU:C	1:B:513:LEU:CD2	2.85	0.50
1:A:390:ASN:HD22	1:A:390:ASN:H	1.60	0.49
1:A:298:ASN:ND2	1:A:302:LYS:HE3	2.27	0.49
1:A:104:HIS:HE1	6:A:1136:HOH:O	1.95	0.49
1:A:381[B]:THR:HG23	6:A:701:HOH:O	2.12	0.49
1:A:333:ASN:HD21	1:A:501:TRP:NE1	2.08	0.49
1:B:511:VAL:O	1:B:515[B]:LYS:HE3	2.13	0.49
1:A:515:LYS:HE2	6:A:837:HOH:O	2.13	0.48
1:B:388:ALA:HB1	1:B:389:THR:HA	1.94	0.48
1:B:195:HIS:HE1	6:B:1164:HOH:O	1.96	0.48
1:B:104:HIS:HE1	6:B:1126:HOH:O	1.96	0.48
1:B:513:LEU:O	1:B:516:VAL:HG12	2.15	0.47
1:A:189:SER:H	1:A:195:HIS:CD2	2.34	0.46
1:B:103:TYR:HB3	1:B:273:TRP:CE3	2.51	0.46
1:B:148:TYR:H	1:B:246:HIS:CE1	2.26	0.46
1:B:298:ASN:ND2	1:B:302:LYS:HE3	2.30	0.46
1:A:388:ALA:HB1	1:A:389:THR:HA	1.98	0.46
1:B:333:ASN:HD21	1:B:501:TRP:NE1	2.14	0.45
1:B:251:SER:O	1:B:269:GLY:HA2	2.17	0.45
1:B:310:HIS:HD2	6:B:1187:HOH:O	2.00	0.45
1:A:29:VAL:H	1:A:467:ASN:ND2	2.15	0.45
1:B:513:LEU:C	1:B:515[B]:LYS:H	2.24	0.45
1:A:103:TYR:HB3	1:A:273:TRP:CE3	2.53	0.44
1:B:349:LEU:HD11	1:B:478:ILE:HG21	2.00	0.43
1:A:390:ASN:ND2	1:A:390:ASN:H	2.17	0.43
1:A:516:VAL:O	1:A:516:VAL:HG22	2.19	0.43
1:B:513:LEU:C	1:B:515[A]:LYS:H	2.26	0.43
1:B:3:SER:HB2	6:B:1122:HOH:O	2.19	0.42
1:B:1:MET:HE2	1:B:2:ALA:H	1.84	0.42
1:A:191:ILE:O	1:A:192:ASP:C	2.61	0.42
1:B:21[B]:LYS:HA	1:B:21[B]:LYS:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LEU:HD21	1:B:462:LYS:HE3	2.01	0.42
1:B:191:ILE:O	1:B:192:ASP:C	2.64	0.41
1:B:413:ALA:HB2	1:B:478:ILE:HG12	2.03	0.41
1:A:520[B]:VAL:HG13	6:A:794:HOH:O	2.19	0.41
1:A:425:HIS:HE1	1:B:225:ASN:HD22	1.69	0.41
1:B:298:ASN:HD21	1:B:302:LYS:HE3	1.86	0.41
1:B:467:ASN:ND2	6:B:715:HOH:O	2.53	0.41
1:A:493:LEU:HD23	1:A:493:LEU:C	2.46	0.40
1:B:170:MET:HE1	1:B:487:ILE:HD11	2.03	0.40
1:A:170:MET:HE1	1:A:487:ILE:HD11	2.04	0.40
1:B:104:HIS:CD2	1:B:104:HIS:H	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:976:HOH:O	6:B:1066:HOH:O[4_455]	2.18	0.02

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	558/555 (100%)	540 (97%)	18 (3%)	0	100	100
1	B	560/555 (101%)	542 (97%)	16 (3%)	2 (0%)	30	12
All	All	1118/1110 (101%)	1082 (97%)	34 (3%)	2 (0%)	44	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	514	GLY
1	B	516	VAL

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	459/463 (99%)	450 (98%)	9 (2%)	50	17
1	B	462/463 (100%)	450 (97%)	12 (3%)	41	10
All	All	921/926 (100%)	900 (98%)	21 (2%)	48	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	VAL
1	A	103	TYR
1	A	195	HIS
1	A	448[A]	LYS
1	A	448[B]	LYS
1	A	508	GLN
1	A	528	LYS
1	A	531	VAL
1	B	1	MET
1	B	103	TYR
1	B	195	HIS
1	B	265	LYS
1	B	423	ASN
1	B	448	LYS
1	B	508	GLN
1	B	513	LEU
1	B	515[A]	LYS
1	B	515[B]	LYS
1	B	516	VAL
1	B	527	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	195	HIS
1	A	225	ASN
1	A	246	HIS
1	A	296	ASN
1	A	309	GLN
1	A	310	HIS
1	A	333	ASN
1	A	350	HIS
1	A	357	GLN
1	A	390	ASN
1	A	392	GLN
1	A	467	ASN
1	A	492	HIS
1	A	502	ASN
1	A	508	GLN
1	B	104	HIS
1	B	124	GLN
1	B	195	HIS
1	B	225	ASN
1	B	246	HIS
1	B	309	GLN
1	B	310	HIS
1	B	333	ASN
1	B	350	HIS
1	B	390	ASN
1	B	392	GLN
1	B	393	HIS
1	B	467	ASN
1	B	492	HIS
1	B	502	ASN
1	B	508	GLN
1	B	544	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 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	A1IIA	B	603	-	11,11,11	1.42	1 (9%)	9,13,13	2.31	1 (11%)
3	A1IIA	A	602	-	11,11,11	1.27	1 (9%)	9,13,13	1.79	2 (22%)
4	A1IH8	B	601	-	10,10,10	1.17	2 (20%)	12,12,12	1.26	2 (16%)
4	A1IH8	A	603	-	10,10,10	1.02	0	12,12,12	1.54	3 (25%)
2	PA5	B	602	-	14,14,14	1.39	2 (14%)	19,20,20	2.82	5 (26%)
2	PA5	A	601	-	14,14,14	0.76	0	19,20,20	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1IIA	B	603	-	-	0/4/8/8	0/1/1/1
3	A1IIA	A	602	-	-	0/4/8/8	0/1/1/1
4	A1IH8	B	601	-	-	0/4/14/14	0/1/1/1
4	A1IH8	A	603	-	-	0/4/14/14	0/1/1/1
2	PA5	B	602	-	-	0/18/18/18	-
2	PA5	A	601	-	-	0/18/18/18	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A1IIA	C06-C05	4.19	1.56	1.51
3	A	602	A1IIA	C06-S10	-3.36	1.66	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	PA5	C4-C3	3.06	1.59	1.53
4	B	601	A1IH8	C02-C01	-2.13	1.47	1.52
4	B	601	A1IH8	C05-C06	2.13	1.58	1.52
2	B	602	PA5	C3-C2	-2.03	1.49	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	PA5	O3-C3-C2	-7.50	95.53	109.21
2	B	602	PA5	O3-C3-C4	5.94	123.15	108.81
3	B	603	A1IIA	C08-C09-S10	-5.78	108.29	112.98
2	B	602	PA5	O2-C2-C3	-4.61	100.68	110.45
2	B	602	PA5	C3-C2-C1	-4.41	103.79	109.32
3	A	602	A1IIA	C08-C09-S10	-4.22	109.56	112.98
4	A	603	A1IH8	C05-C04-C03	-2.85	107.71	112.42
4	B	601	A1IH8	C04-C05-C06	-2.69	107.96	112.42
3	A	602	A1IIA	C07-C06-C05	-2.49	126.10	129.02
4	B	601	A1IH8	C02-C01-C06	2.13	115.94	112.42
4	A	603	A1IH8	C04-C05-C06	-2.06	109.00	112.42
2	B	602	PA5	C5-C4-C3	2.03	116.13	112.20
4	A	603	A1IH8	C01-C02-C03	2.02	115.77	112.42

There are no chirality outliers.

There are no torsion outliers.

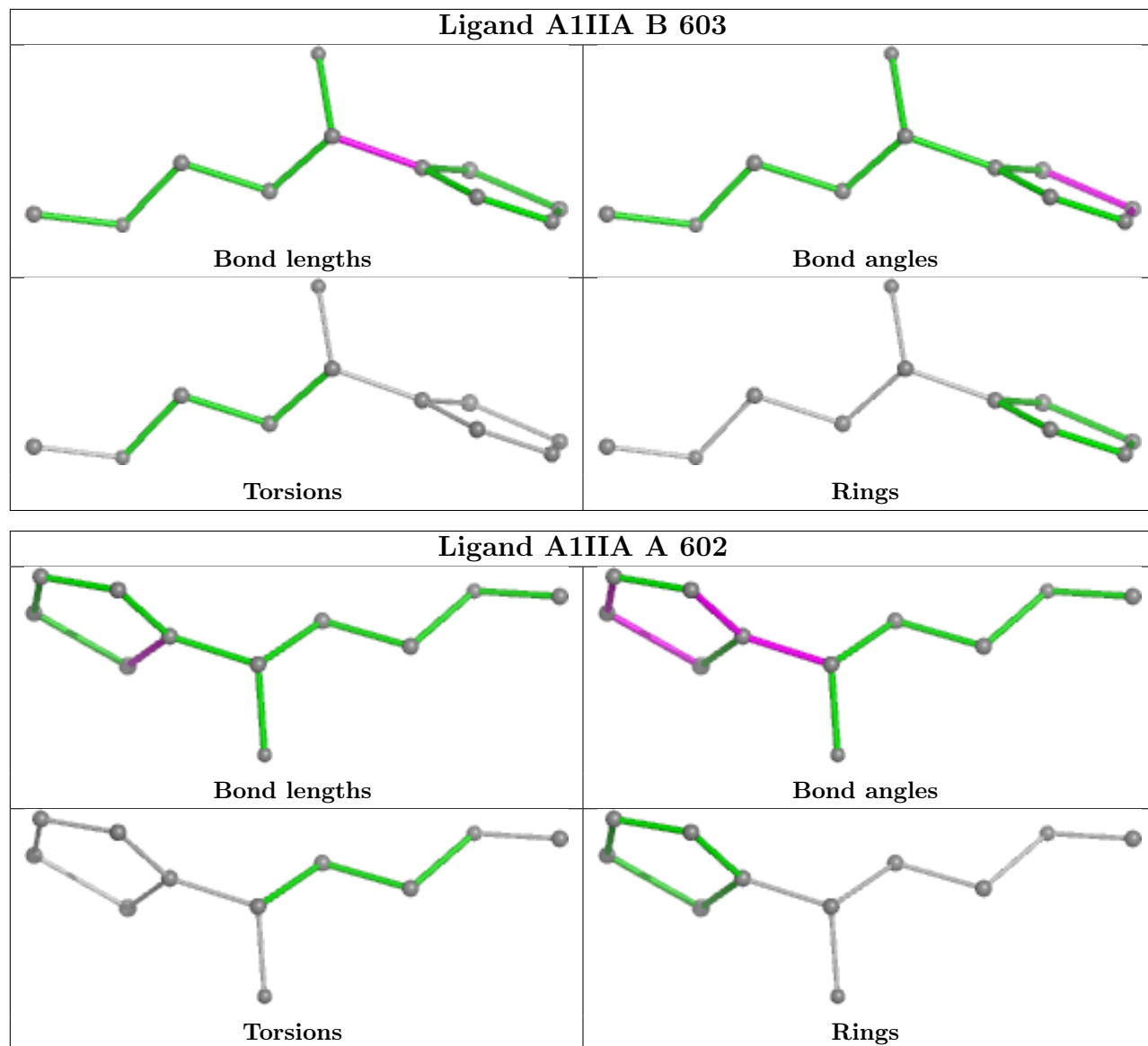
There are no ring outliers.

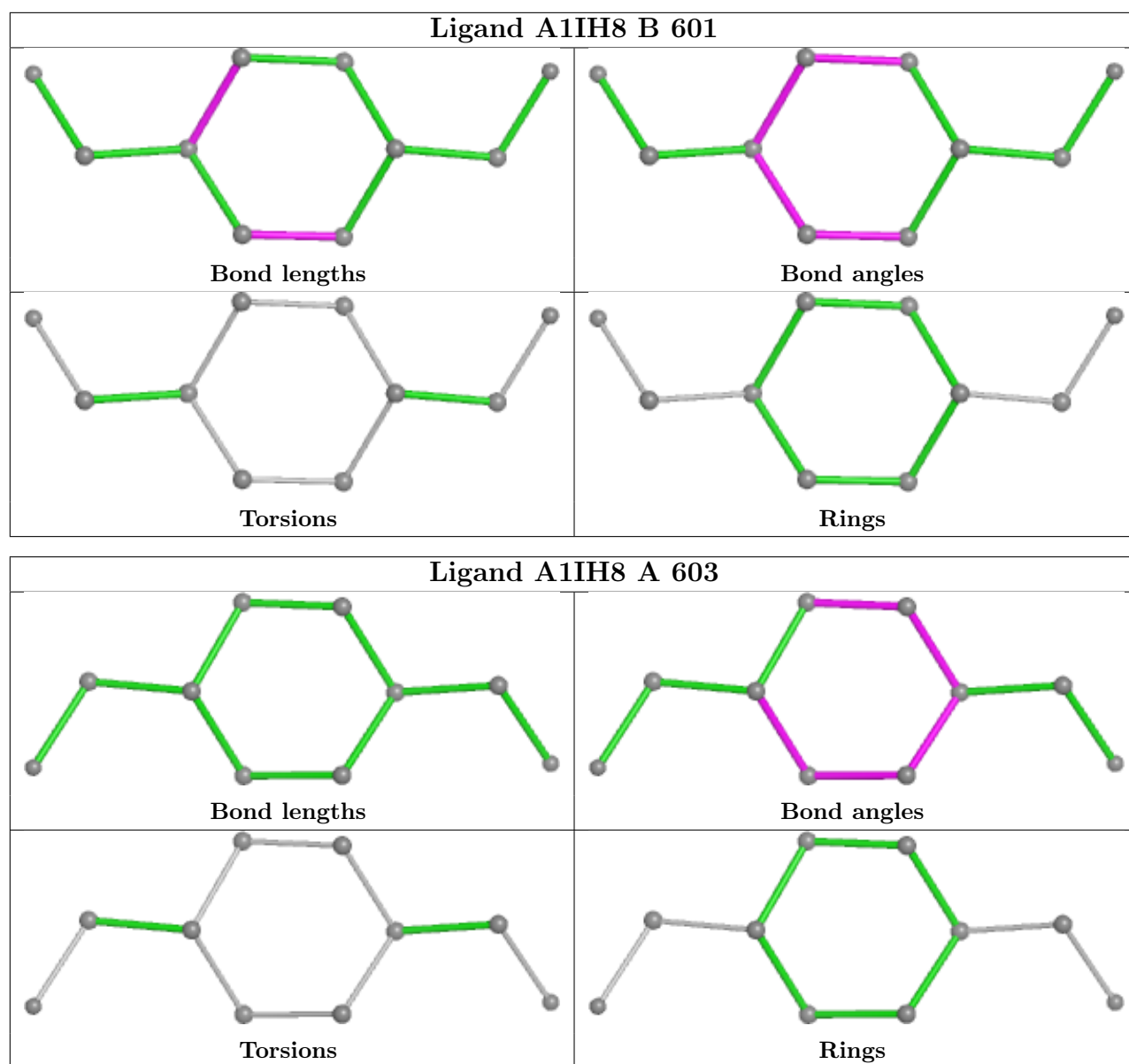
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PA5	1	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	550/555 (99%)	-0.37	6 (1%) 77 81	7, 11, 23, 50	10 (1%)
1	B	550/555 (99%)	-0.30	13 (2%) 59 60	6, 11, 23, 59	12 (2%)
All	All	1100/1110 (99%)	-0.34	19 (1%) 69 71	6, 11, 23, 59	22 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	VAL	10.4
1	B	515[A]	LYS	6.2
1	B	517	LEU	5.3
1	B	514	GLY	5.0
1	B	513	LEU	4.3
1	B	527	ASP	4.2
1	A	1	MET	4.1
1	B	511	VAL	4.0
1	A	394	SER	3.8
1	A	527	ASP	3.7
1	B	1	MET	2.8
1	A	550	GLU	2.6
1	A	528	LYS	2.4
1	B	201	LYS	2.4
1	A	516	VAL	2.3
1	B	512	GLU	2.3
1	B	262	ILE	2.3
1	B	259	ALA	2.1
1	B	526	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

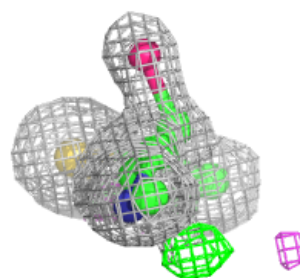
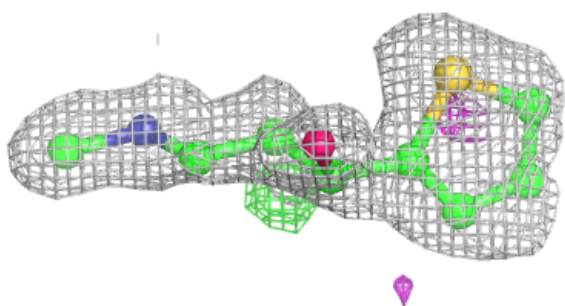
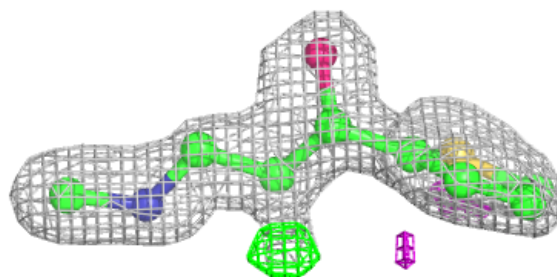
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1IIA	B	603	11/11	0.85	0.13	26,32,34,36	0
3	A1IIA	A	602	11/11	0.89	0.12	23,27,29,31	0
2	PA5	B	602	15/15	0.91	0.09	19,21,24,24	0
4	A1IH8	A	603	10/10	0.92	0.08	16,17,20,21	0
4	A1IH8	B	601	10/10	0.92	0.09	21,22,24,28	0
2	PA5	A	601	15/15	0.98	0.04	11,12,14,14	0
5	CL	A	604	1/1	0.99	0.09	20,20,20,20	0
5	CL	B	604	1/1	1.00	0.15	20,20,20,20	0

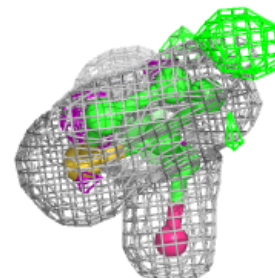
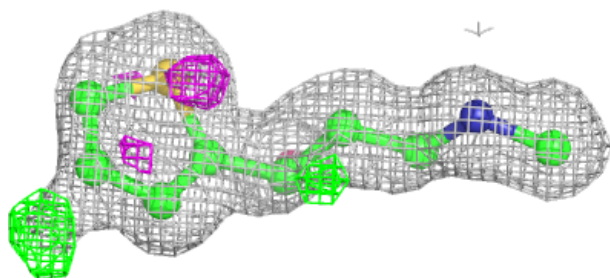
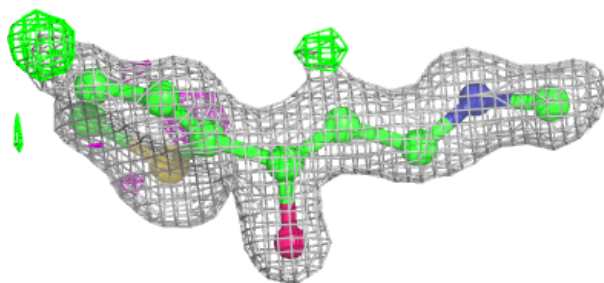
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IIA 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)

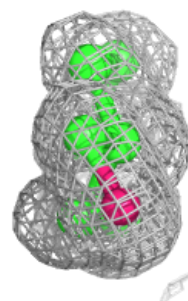
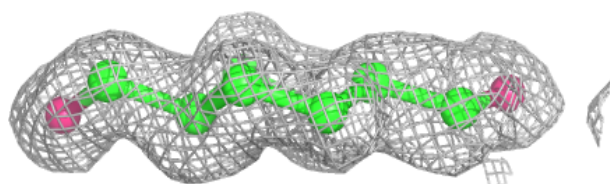
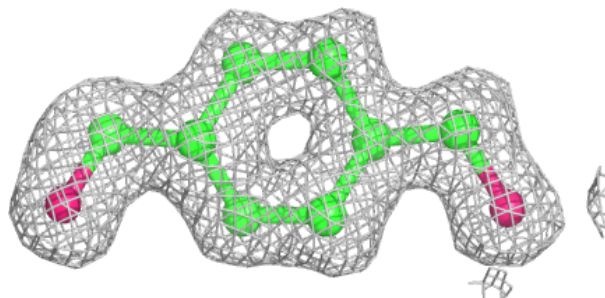
**Electron density around A1IIA A 602:**

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

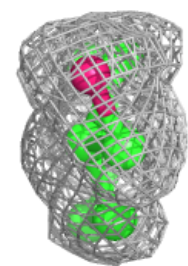
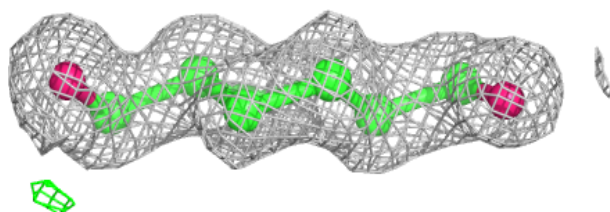
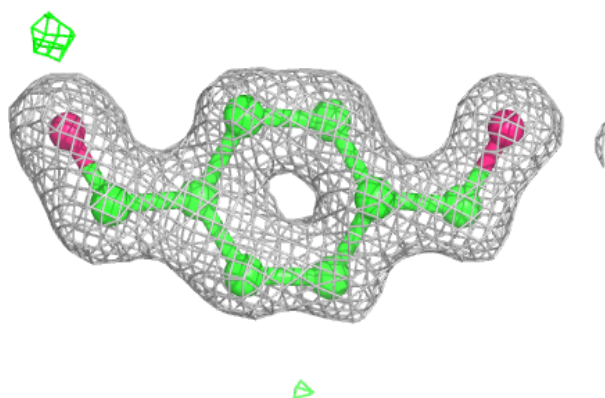


Electron density around A1IH8 A 603:

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

**Electron density around A1IH8 B 601:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.