



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2022 – 06:16 pm GMT

PDB ID : 7ZHZ
Title : Leishmania donovani Glucose 6-Phosphate Dehydrogenase mutant C138S complexed with G6P and NADP(H)
Authors : Fritz-Wolf, K.; Berneburg, I.
Deposited on : 2022-04-07
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

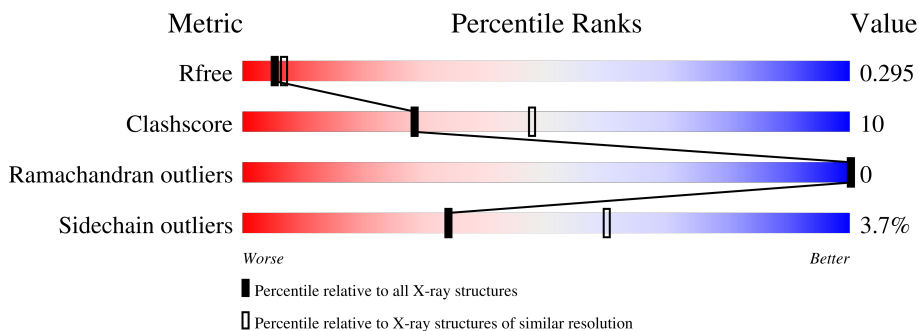
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	562	 72% 22% • 6%
1	B	562	 67% 26% • 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	605	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8532 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.

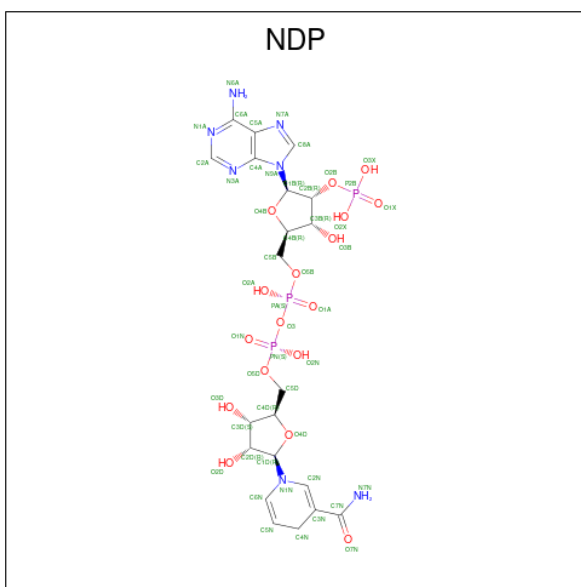
- Molecule 1 is a protein called Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	528	Total 4172	C 2652	N 714	O 790	S 16	0	0	0
1	B	527	Total 4172	C 2654	N 717	O 786	S 15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	SER	CYS	engineered mutation	UNP A2CIL3
B	138	SER	CYS	engineered mutation	UNP A2CIL3

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



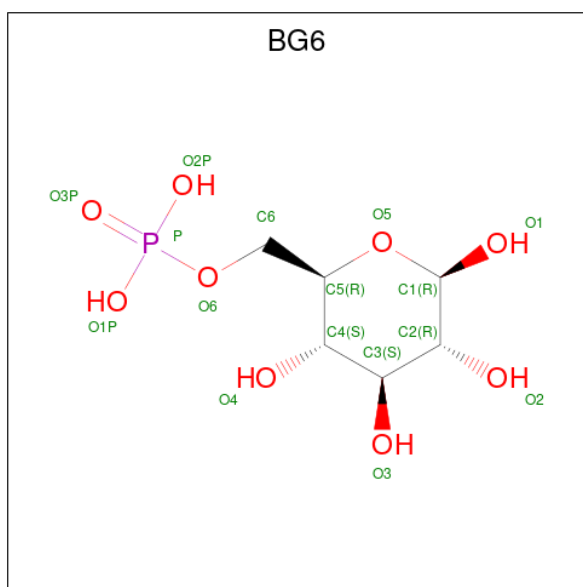
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula: $C_6H_{13}O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	B	1	16	6	9	1	0	0

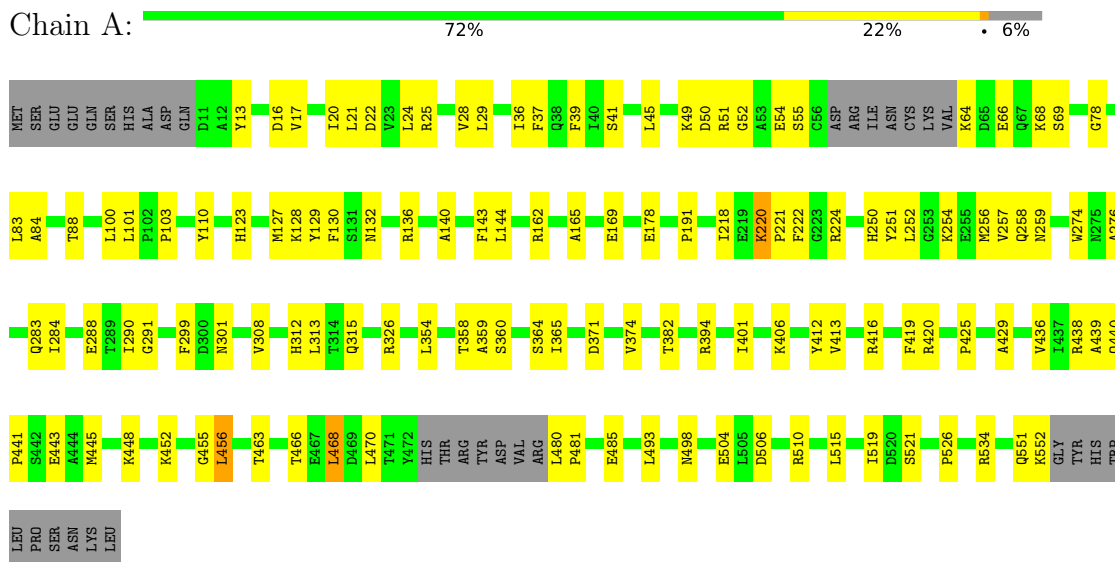
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	15	15	15	0	0
6	B	10	10	10	0	0

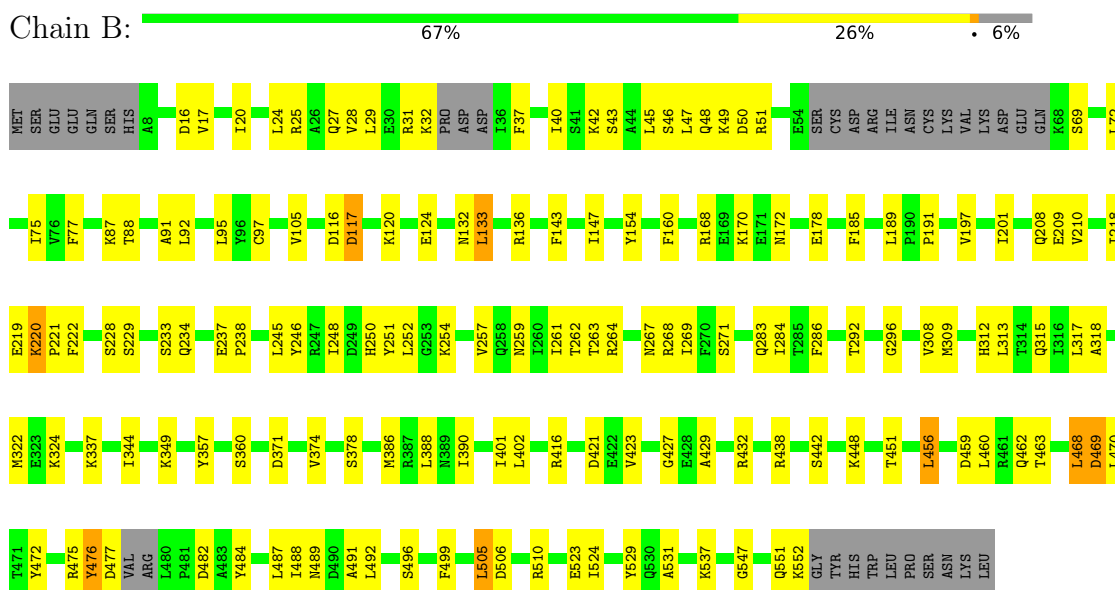
3 Residue-property plots

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. 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. 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 1-dehydrogenase



- Molecule 1: Glucose-6-phosphate 1-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.16Å 66.02Å 120.02Å 90.00° 120.73° 90.00°	Depositor
Resolution (Å)	48.75 – 2.50 48.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.75-2.50) 99.7 (48.75-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.249 , 0.298 0.245 , 0.295	Depositor DCC
R_{free} test set	5105 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtrriage
Anisotropy	0.493	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.004 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, BG6, SO4, 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	0.25	0/4257	0.51	1/5755 (0.0%)
1	B	0.27	0/4257	0.52	1/5754 (0.0%)
All	All	0.26	0/8514	0.52	2/11509 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	468	LEU	CA-CB-CG	7.28	132.04	115.30
1	B	468	LEU	CA-CB-CG	6.09	129.31	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	476	TYR	Peptide

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	4172	0	4143	77	0
1	B	4172	0	4143	101	0
2	A	48	0	26	1	0
2	B	48	0	26	1	0
3	A	8	0	12	1	0
3	B	8	0	12	1	0
4	A	15	0	0	2	0
4	B	20	0	0	2	0
5	B	16	0	11	0	0
6	A	15	0	0	1	0
6	B	10	0	0	2	0
All	All	8532	0	8373	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (166) 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:220:LYS:NZ	6:B:701:HOH:O	2.15	0.79
1:B:69:SER:OG	1:B:178:GLU:OE2	2.00	0.78
1:B:421:ASP:HB2	1:B:432:ARG:HG2	1.67	0.75
1:A:452:LYS:HB2	1:B:262:THR:HG21	1.71	0.73
1:B:250:HIS:ND1	6:B:701:HOH:O	2.22	0.71
1:A:127:MET:HA	1:A:130:PHE:CD1	2.27	0.70
1:B:318:ALA:HB1	1:B:337:LYS:HB2	1.75	0.69
1:B:252:LEU:HD21	1:B:315:GLN:HB3	1.75	0.69
1:A:22:ASP:HB3	1:A:25:ARG:HH21	1.58	0.69
1:A:21:LEU:HA	1:A:24:LEU:HD23	1.77	0.66
1:A:254:LYS:HG2	1:A:439:ALA:HB1	1.78	0.66
1:A:480:LEU:HB3	1:A:481:PRO:HD3	1.77	0.64
1:B:25:ARG:NH2	1:B:124:GLU:OE2	2.32	0.63
1:B:309:MET:HE3	1:B:313:LEU:HD12	1.81	0.63
1:A:429:ALA:O	1:A:463:THR:OG1	2.16	0.63
1:B:237:GLU:HG3	1:B:238:PRO:HD3	1.81	0.61
1:B:308:VAL:HG23	1:B:312:HIS:HD2	1.65	0.61
1:B:448:LYS:NZ	4:B:605:SO4:O3	2.33	0.61
1:A:251:TYR:HE2	1:A:413:VAL:HG11	1.64	0.61
1:A:16:ASP:O	1:A:20:ILE:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:SER:HB3	1:A:178:GLU:OE2	2.01	0.60
1:A:218:ILE:HG22	1:A:222:PHE:HE2	1.64	0.60
1:B:484:TYR:HA	1:B:487:LEU:HD12	1.83	0.60
1:A:551:GLN:O	1:A:552:LYS:HB2	2.01	0.60
1:B:484:TYR:O	1:B:487:LEU:N	2.35	0.59
1:A:274:TRP:O	1:A:394:ARG:NH1	2.35	0.59
1:B:349:LYS:HB2	1:B:524:ILE:HD11	1.84	0.59
1:A:299:PHE:HE2	1:A:382:THR:HG22	1.68	0.59
1:B:91:ALA:O	1:B:95:LEU:HD12	2.02	0.59
1:A:468:LEU:HB3	1:B:468:LEU:CD1	2.33	0.58
1:A:468:LEU:HD13	1:B:470:LEU:HA	1.87	0.57
1:B:16:ASP:OD1	1:B:17:VAL:N	2.38	0.57
1:B:168:ARG:O	1:B:172:ASN:ND2	2.35	0.57
1:B:28:VAL:HG13	1:B:29:LEU:HD22	1.87	0.57
1:B:222:PHE:O	1:B:229:SER:OG	2.22	0.56
1:B:88:THR:O	1:B:92:LEU:HD12	2.05	0.56
1:B:219:GLU:HG3	1:B:220:LYS:H	1.69	0.56
1:A:254:LYS:NZ	3:A:602:EDO:O1	2.36	0.56
1:B:416:ARG:NH2	4:B:605:SO4:O3	2.39	0.56
1:B:117:ASP:HB3	1:B:120:LYS:HB3	1.87	0.55
1:B:489:ASN:HA	1:B:492:LEU:HD12	1.87	0.55
1:B:48:GLN:HG3	1:B:49:LYS:H	1.71	0.55
1:B:208:GLN:HG2	1:B:210:VAL:HG22	1.90	0.54
1:A:17:VAL:HA	1:A:20:ILE:HB	1.90	0.54
1:A:283:GLN:HG3	1:A:401:ILE:HB	1.90	0.54
1:B:259:ASN:OD1	1:B:262:THR:OG1	2.25	0.54
1:B:360:SER:HB3	1:B:531:ALA:HB3	1.90	0.54
1:A:252:LEU:HB3	1:A:498:ASN:HB3	1.90	0.54
1:B:37:PHE:HA	1:B:40:ILE:HD12	1.89	0.54
1:B:438:ARG:NH1	1:B:442:SER:O	2.36	0.54
1:B:48:GLN:HG3	1:B:49:LYS:N	2.23	0.54
1:B:484:TYR:O	1:B:488:ILE:HD12	2.09	0.53
1:A:36:ILE:HG22	1:A:39:PHE:H	1.73	0.53
1:A:78:GLY:N	1:A:110:TYR:O	2.41	0.53
1:A:251:TYR:CE2	1:A:413:VAL:HG11	2.43	0.52
1:B:229:SER:HB3	1:B:505:LEU:HD21	1.91	0.52
1:B:97:CYS:SG	1:B:136:ARG:NH2	2.76	0.52
1:B:292:THR:HG21	1:B:296:GLY:HA2	1.92	0.52
1:A:68:LYS:HE3	1:A:103:PRO:HD3	1.92	0.52
1:B:456:LEU:N	1:B:456:LEU:HD13	2.25	0.52
1:B:43:SER:O	1:B:47:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:PRO:HG3	1:B:324:LYS:HE2	1.92	0.51
1:A:128:LYS:HE3	1:A:129:TYR:CE2	2.46	0.51
1:B:218:ILE:O	1:B:248:ILE:HG22	2.11	0.51
1:B:264:ARG:NH1	1:B:322:MET:O	2.43	0.51
1:B:459:ASP:H	1:B:462:GLN:HG3	1.75	0.51
1:A:84:ALA:HA	1:A:88:THR:HB	1.94	0.50
1:A:49:LYS:HE3	1:A:52:GLY:HA3	1.94	0.50
1:A:50:ASP:O	1:A:54:GLU:HG3	2.11	0.50
1:A:224:ARG:NH2	1:A:301:ASN:O	2.31	0.50
1:B:551:GLN:HG2	1:B:552:LYS:N	2.27	0.50
1:A:218:ILE:HG22	1:A:222:PHE:CE2	2.46	0.50
1:B:344:ILE:HG21	1:B:388:LEU:HD23	1.93	0.50
1:B:222:PHE:HB2	1:B:505:LEU:HD11	1.93	0.50
1:A:127:MET:HA	1:A:130:PHE:CE1	2.47	0.50
1:A:64:LYS:HE3	1:A:493:LEU:HD21	1.94	0.49
1:B:309:MET:CE	1:B:402:LEU:HB3	2.43	0.49
1:B:16:ASP:O	1:B:20:ILE:HG12	2.12	0.49
1:B:432:ARG:NH2	1:B:547:GLY:O	2.34	0.49
1:B:284:ILE:HG22	1:B:313:LEU:HD22	1.94	0.49
1:A:420:ARG:NH1	4:A:604:SO4:O1	2.45	0.48
1:B:429:ALA:O	1:B:463:THR:OG1	2.22	0.48
1:B:31:ARG:HE	1:B:32:LYS:H	1.60	0.48
1:B:77:PHE:HB3	1:B:189:LEU:HD11	1.96	0.48
1:B:261:ILE:HD12	1:B:261:ILE:H	1.78	0.48
1:A:37:PHE:CE2	1:B:475:ARG:HD3	2.49	0.48
1:A:127:MET:HA	1:A:130:PHE:HD1	1.76	0.47
1:A:468:LEU:HB3	1:B:468:LEU:HD12	1.95	0.47
1:B:268:ARG:HH22	3:B:601:EDO:H22	1.79	0.47
1:A:290:ILE:HD12	1:A:291:GLY:O	2.14	0.47
1:A:276:ALA:N	1:A:394:ARG:O	2.47	0.47
1:A:220:LYS:HE2	1:A:250:HIS:CE1	2.49	0.46
1:B:72:LEU:HD23	1:B:105:VAL:HG23	1.97	0.46
1:A:506:ASP:O	1:A:510:ARG:HG3	2.16	0.46
1:A:191:PRO:HG3	1:A:221:PRO:HD2	1.96	0.46
1:A:140:ALA:HA	1:A:143:PHE:HB3	1.98	0.46
1:A:254:LYS:O	1:A:258:GLN:HG3	2.15	0.46
1:B:317:LEU:HD21	1:B:390:ILE:HD11	1.97	0.46
1:B:459:ASP:N	1:B:462:GLN:HG3	2.31	0.46
1:A:132:ASN:OD1	1:A:136:ARG:NH2	2.49	0.45
1:B:469:ASP:OD2	1:B:469:ASP:N	2.48	0.45
1:A:440:GLN:HG3	1:A:441:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:TYR:HB3	1:B:197:VAL:HG22	1.99	0.45
1:B:47:LEU:HA	1:B:50:ASP:HB2	1.98	0.45
1:A:466:THR:OG1	1:B:472:TYR:HB2	2.16	0.45
1:A:425:PRO:HD3	1:B:324:LYS:NZ	2.31	0.45
1:B:506:ASP:O	1:B:510:ARG:HG3	2.17	0.45
1:A:358:THR:OG1	1:A:359:ALA:N	2.48	0.45
1:B:27:GLN:NE2	1:B:133:LEU:HD13	2.32	0.44
1:A:259:ASN:HD21	1:B:451:THR:HB	1.81	0.44
1:B:551:GLN:O	1:B:552:LYS:HB2	2.18	0.44
1:B:170:LYS:HE2	1:B:170:LYS:HB2	1.83	0.44
1:B:357:TYR:HA	1:B:529:TYR:O	2.17	0.44
1:B:537:LYS:HD3	1:B:537:LYS:HA	1.76	0.44
1:B:75:ILE:HD13	1:B:185:PHE:CE1	2.53	0.44
1:A:468:LEU:HB3	1:B:468:LEU:HD13	1.99	0.44
1:B:191:PRO:HG3	1:B:221:PRO:HB2	1.99	0.44
1:B:263:THR:HA	1:B:267:ASN:ND2	2.33	0.44
1:B:317:LEU:HD12	1:B:402:LEU:HD11	1.98	0.44
1:A:315:GLN:NE2	1:A:504:GLU:OE2	2.37	0.44
1:B:283:GLN:HG3	1:B:401:ILE:HB	2.00	0.44
1:A:25:ARG:O	1:A:28:VAL:HG12	2.18	0.43
1:A:412:TYR:CE1	1:A:438:ARG:HD3	2.52	0.43
1:A:416:ARG:HG3	1:A:436:VAL:HG22	1.99	0.43
1:B:308:VAL:O	1:B:312:HIS:HB2	2.18	0.43
1:B:251:TYR:OH	1:B:286:PHE:HE2	2.01	0.43
1:B:551:GLN:HG2	1:B:552:LYS:H	1.84	0.43
1:A:448:LYS:NZ	6:A:702:HOH:O	2.51	0.43
1:A:354:LEU:HB2	1:A:526:PRO:HA	2.00	0.43
1:B:254:LYS:HB2	1:B:257:VAL:HG22	2.01	0.43
1:A:284:ILE:HG22	1:A:313:LEU:HD22	2.00	0.43
1:A:288:GLU:OE2	1:A:406:LYS:NZ	2.52	0.43
1:A:552:LYS:HD3	1:A:552:LYS:HA	1.88	0.43
1:B:143:PHE:CZ	1:B:147:ILE:HD11	2.53	0.43
1:B:160:PHE:HE2	1:B:201:ILE:HG13	1.83	0.43
1:B:496:SER:HA	1:B:499:PHE:HD2	1.83	0.43
1:A:83:LEU:HD13	2:A:601:NDP:H2N	1.99	0.42
1:A:256:MET:HG2	1:A:443:GLU:CD	2.39	0.42
1:A:470:LEU:HA	1:B:468:LEU:HA	2.00	0.42
1:A:515:LEU:O	1:A:519:ILE:HG12	2.19	0.42
1:B:45:LEU:O	1:B:48:GLN:HG2	2.20	0.42
1:A:308:VAL:O	1:A:312:HIS:HB2	2.19	0.42
1:A:481:PRO:HB2	1:A:485:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HE	1:B:32:LYS:N	2.17	0.42
1:B:218:ILE:HD11	1:B:245:LEU:HD22	2.01	0.42
1:A:165:ALA:O	1:A:169:GLU:HG3	2.20	0.42
1:B:246:TYR:CE1	1:B:491:ALA:HA	2.54	0.42
1:A:123:HIS:O	1:A:127:MET:HB2	2.20	0.41
1:A:534:ARG:NH2	4:A:605:SO4:O2	2.53	0.41
1:B:132:ASN:OD1	1:B:132:ASN:N	2.51	0.41
1:B:476:TYR:O	1:B:477:ASP:HB3	2.20	0.41
1:A:360:SER:OG	1:A:365:ILE:N	2.44	0.41
1:A:455:GLY:O	1:A:456:LEU:HD22	2.21	0.41
1:B:423:VAL:HG23	1:B:427:GLY:HA2	2.03	0.41
1:B:523:GLU:C	1:B:524:ILE:HD13	2.40	0.41
1:A:100:LEU:O	1:A:101:LEU:HD23	2.21	0.41
1:A:140:ALA:O	1:A:144:LEU:HG	2.21	0.41
1:A:412:TYR:HE1	1:A:438:ARG:HD3	1.86	0.41
1:B:228:SER:H	1:B:228:SER:HG	1.66	0.41
1:B:220:LYS:HB2	2:B:602:NDP:H6N	2.03	0.41
1:B:259:ASN:HD21	1:B:263:THR:CG2	2.34	0.40
1:A:419:PHE:CE2	1:B:269:ILE:HD11	2.56	0.40
1:B:371:ASP:HB3	1:B:374:VAL:HG23	2.02	0.40
1:A:254:LYS:O	1:A:257:VAL:HG22	2.21	0.40
1:A:371:ASP:HB3	1:A:374:VAL:HG13	2.04	0.40
1:B:234:GLN:HA	1:B:237:GLU:HG2	2.03	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	522/562 (93%)	501 (96%)	21 (4%)	0	100 100
1	B	519/562 (92%)	502 (97%)	17 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1041/1124 (93%)	1003 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	450/482 (93%)	436 (97%)	14 (3%)	40	67
1	B	448/482 (93%)	429 (96%)	19 (4%)	30	54
All	All	898/964 (93%)	865 (96%)	33 (4%)	34	60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	TYR
1	A	29	LEU
1	A	41	SER
1	A	45	LEU
1	A	51	ARG
1	A	55	SER
1	A	66	GLU
1	A	162	ARG
1	A	220	LYS
1	A	326	ARG
1	A	364	SER
1	A	445	MET
1	A	456	LEU
1	A	521	SER
1	B	24	LEU
1	B	42	LYS
1	B	46	SER
1	B	51	ARG
1	B	87	LYS
1	B	116	ASP

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Mol	Chain	Res	Type
1	B	117	ASP
1	B	133	LEU
1	B	209	GLU
1	B	220	LYS
1	B	233	SER
1	B	271	SER
1	B	378	SER
1	B	386	MET
1	B	456	LEU
1	B	460	LEU
1	B	469	ASP
1	B	482	ASP
1	B	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	HIS
1	B	27	GLN
1	B	312	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](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	605	-	4,4,4	0.14	0	6,6,6	0.04	0
3	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.34	0
4	SO4	B	607	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	606	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	B	603	-	3,3,3	0.45	0	2,2,2	0.34	0
4	SO4	B	608	-	4,4,4	0.14	0	6,6,6	0.05	0
3	EDO	B	601	-	3,3,3	0.46	0	2,2,2	0.33	0
5	BG6	B	604	-	16,16,16	1.23	2 (12%)	24,24,24	1.17	3 (12%)
2	NDP	B	602	-	45,52,52	4.02	18 (40%)	53,80,80	2.27	5 (9%)
4	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.05	0
2	NDP	A	601	-	45,52,52	4.01	18 (40%)	53,80,80	2.30	6 (11%)

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	EDO	A	602	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	B	601	-	-	0/1/1/1	-
5	BG6	B	604	-	-	2/6/26/26	0/1/1/1
2	NDP	B	602	-	-	9/30/77/77	0/5/5/5
2	NDP	A	601	-	-	6/30/77/77	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NDP	O4B-C1B	13.68	1.60	1.41
2	A	601	NDP	O4B-C1B	13.67	1.60	1.41
2	A	601	NDP	C6N-C5N	12.69	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NDP	C6N-C5N	12.66	1.55	1.33
2	B	602	NDP	O4D-C1D	7.80	1.60	1.42
2	A	601	NDP	O4D-C1D	7.74	1.60	1.42
2	B	602	NDP	C2D-C1D	-7.15	1.30	1.53
2	A	601	NDP	C2D-C1D	-7.14	1.30	1.53
2	B	602	NDP	O4D-C4D	-6.78	1.29	1.45
2	A	601	NDP	O4D-C4D	-6.70	1.30	1.45
2	A	601	NDP	O4B-C4B	-6.30	1.30	1.45
2	B	602	NDP	O4B-C4B	-6.28	1.31	1.45
2	B	602	NDP	C2N-C3N	5.26	1.49	1.34
2	A	601	NDP	C2N-C3N	5.20	1.49	1.34
2	A	601	NDP	O2D-C2D	4.40	1.53	1.43
2	B	602	NDP	O2D-C2D	4.38	1.53	1.43
2	B	602	NDP	P2B-O2B	4.35	1.67	1.59
2	A	601	NDP	P2B-O2B	4.31	1.67	1.59
2	B	602	NDP	C4N-C3N	4.17	1.58	1.49
2	A	601	NDP	C4N-C3N	4.14	1.58	1.49
2	A	601	NDP	C7N-N7N	3.51	1.42	1.33
2	B	602	NDP	C7N-N7N	3.51	1.42	1.33
2	B	602	NDP	C6N-N1N	3.34	1.45	1.37
2	A	601	NDP	C6N-N1N	3.34	1.45	1.37
2	B	602	NDP	C6A-N6A	3.30	1.46	1.34
2	A	601	NDP	C6A-N6A	3.29	1.46	1.34
5	B	604	BG6	O5-C1	3.09	1.50	1.42
2	A	601	NDP	C4N-C5N	2.91	1.56	1.48
2	B	602	NDP	C5D-C4D	2.89	1.60	1.51
2	B	602	NDP	C4N-C5N	2.88	1.56	1.48
2	A	601	NDP	C5D-C4D	2.80	1.60	1.51
2	A	601	NDP	C5A-C4A	-2.51	1.34	1.40
2	B	602	NDP	C5A-C4A	-2.50	1.34	1.40
2	A	601	NDP	C2A-N3A	2.47	1.36	1.32
2	B	602	NDP	C2A-N3A	2.47	1.36	1.32
2	A	601	NDP	PA-O5B	2.08	1.67	1.59
2	B	602	NDP	PA-O5B	2.07	1.67	1.59
5	B	604	BG6	P-O6	2.03	1.66	1.60

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NDP	C5A-C6A-N6A	9.92	135.43	120.35
2	B	602	NDP	C5A-C6A-N6A	9.91	135.42	120.35
2	A	601	NDP	C1B-N9A-C4A	-8.49	111.72	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NDP	C1B-N9A-C4A	-8.43	111.83	126.64
2	A	601	NDP	N6A-C6A-N1A	-6.74	104.59	118.57
2	B	602	NDP	N6A-C6A-N1A	-6.72	104.61	118.57
2	A	601	NDP	N3A-C2A-N1A	-5.53	120.04	128.68
2	B	602	NDP	N3A-C2A-N1A	-5.50	120.08	128.68
2	A	601	NDP	PN-O3-PA	-2.80	123.21	132.83
2	B	602	NDP	PN-O3-PA	-2.60	123.89	132.83
5	B	604	BG6	C4-C3-C2	2.55	115.28	110.82
5	B	604	BG6	C3-C4-C5	2.40	114.53	110.24
5	B	604	BG6	C6-C5-C4	-2.20	107.49	112.09
2	A	601	NDP	C3D-C2D-C1D	2.03	105.28	101.43

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NDP	C5D-O5D-PN-O1N
2	A	601	NDP	O4D-C1D-N1N-C6N
2	B	602	NDP	C5D-O5D-PN-O1N
5	B	604	BG6	O5-C5-C6-O6
5	B	604	BG6	C4-C5-C6-O6
2	A	601	NDP	PN-O3-PA-O1A
2	B	602	NDP	C2B-O2B-P2B-O3X
2	B	602	NDP	C5D-O5D-PN-O3
2	B	602	NDP	C2D-C1D-N1N-C6N
2	B	602	NDP	O4D-C1D-N1N-C6N
2	B	602	NDP	PN-O3-PA-O1A
2	B	602	NDP	C2D-C1D-N1N-C2N
2	A	601	NDP	O4D-C4D-C5D-O5D
2	B	602	NDP	O4D-C1D-N1N-C2N
2	A	601	NDP	C2B-O2B-P2B-O2X
2	A	601	NDP	C2B-O2B-P2B-O3X
2	B	602	NDP	C2B-O2B-P2B-O2X

There are no ring outliers.

7 monomers are involved in 8 short contacts:

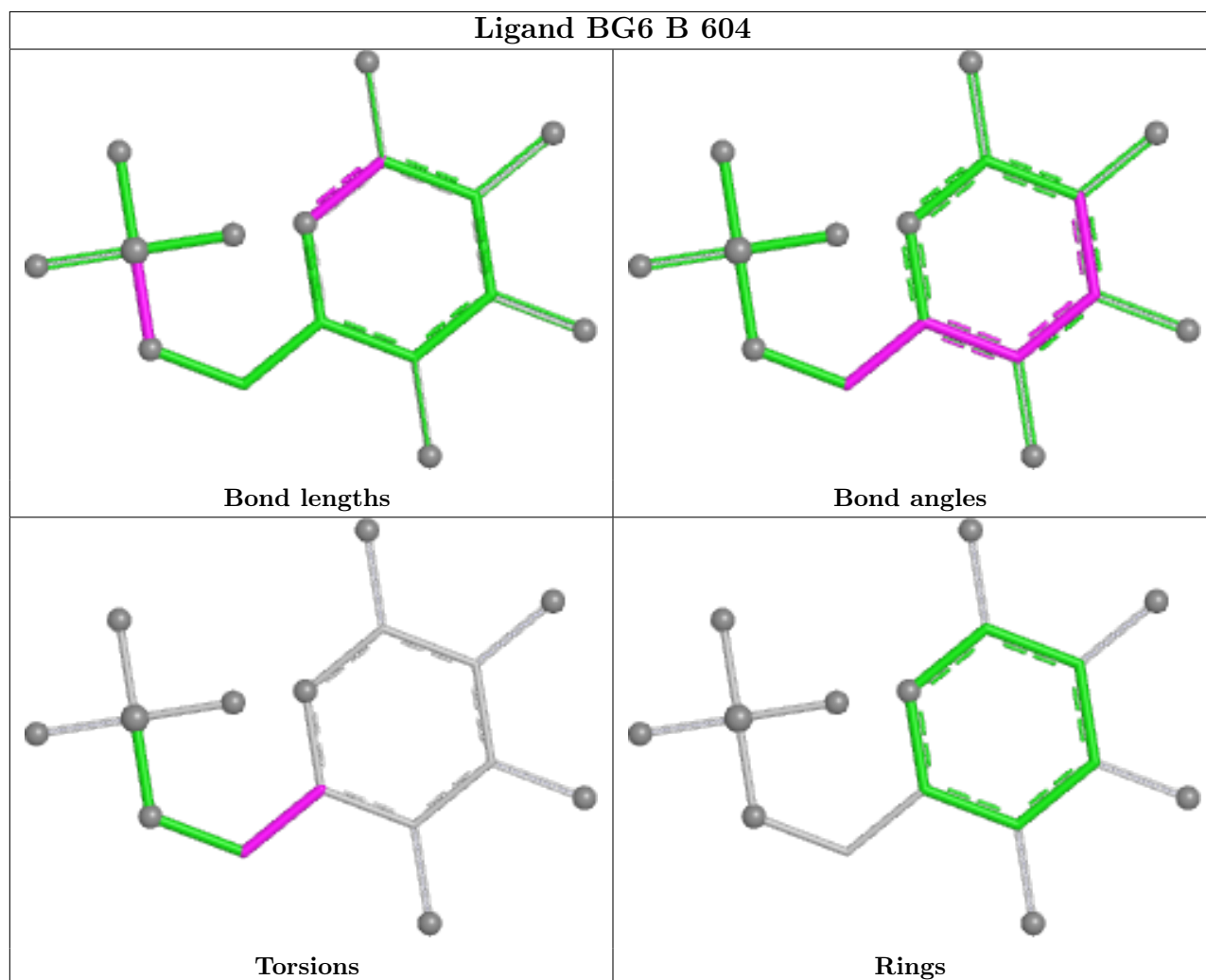
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	SO4	2	0
3	A	602	EDO	1	0
4	A	604	SO4	1	0

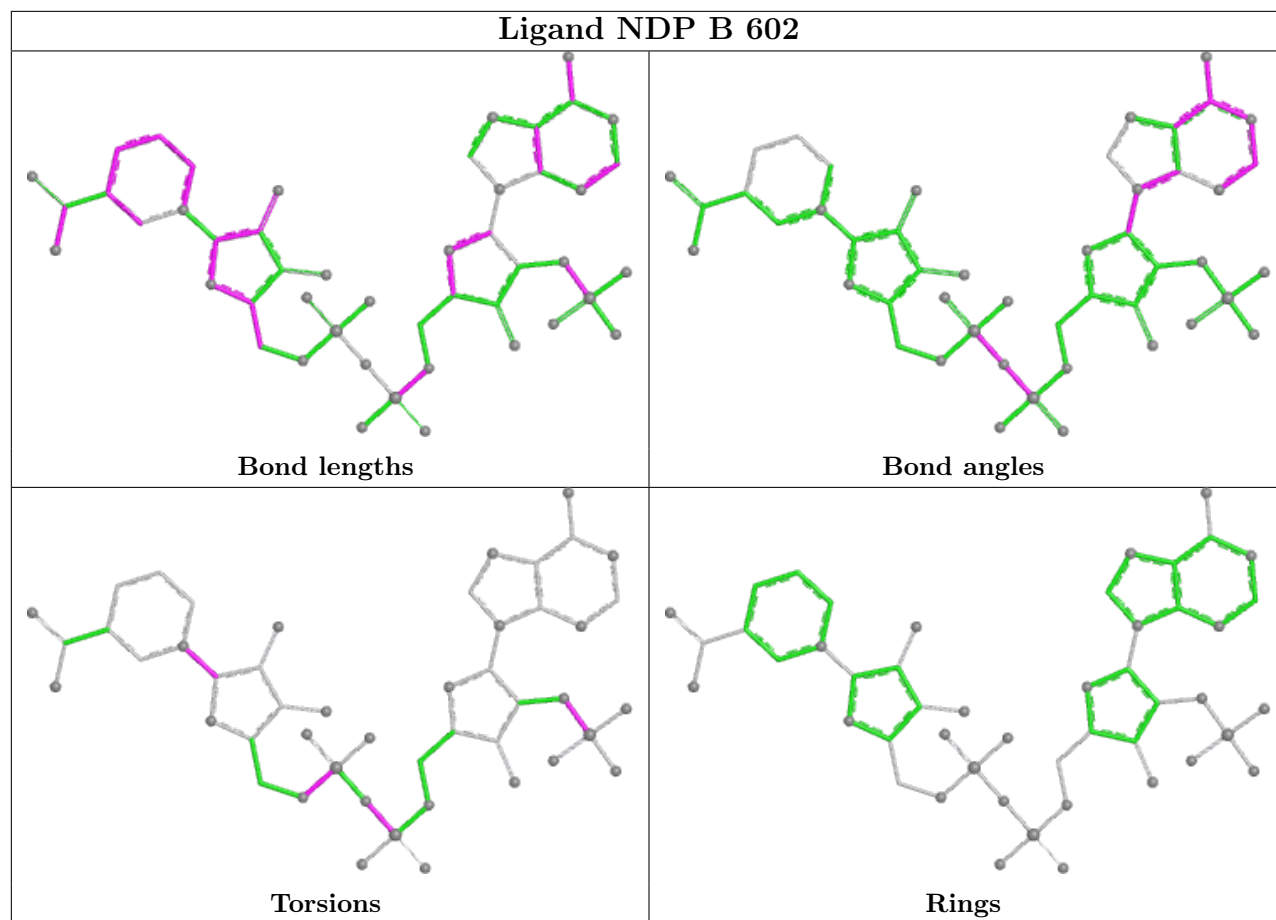
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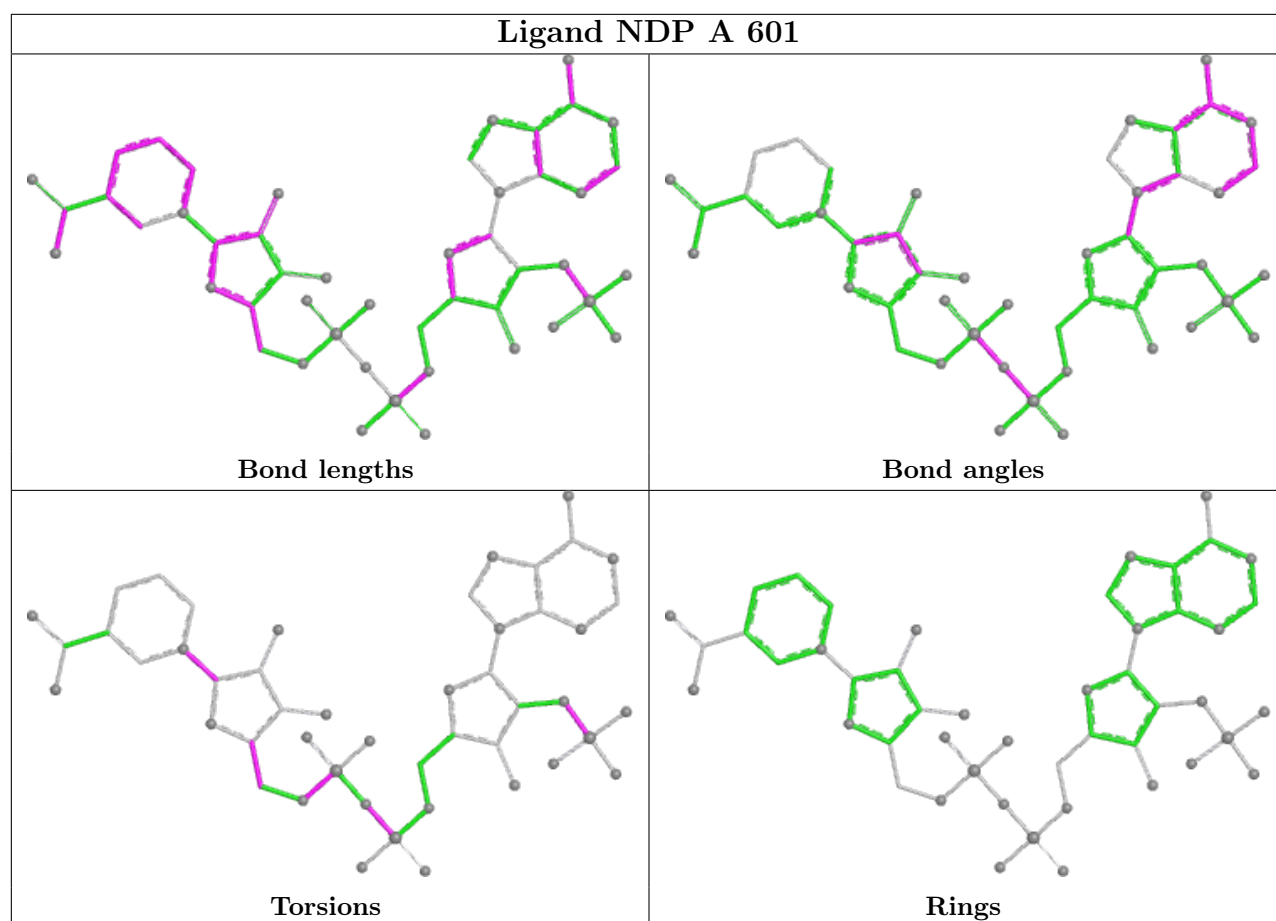
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	EDO	1	0
2	B	602	NDP	1	0
4	A	605	SO4	1	0
2	A	601	NDP	1	0

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

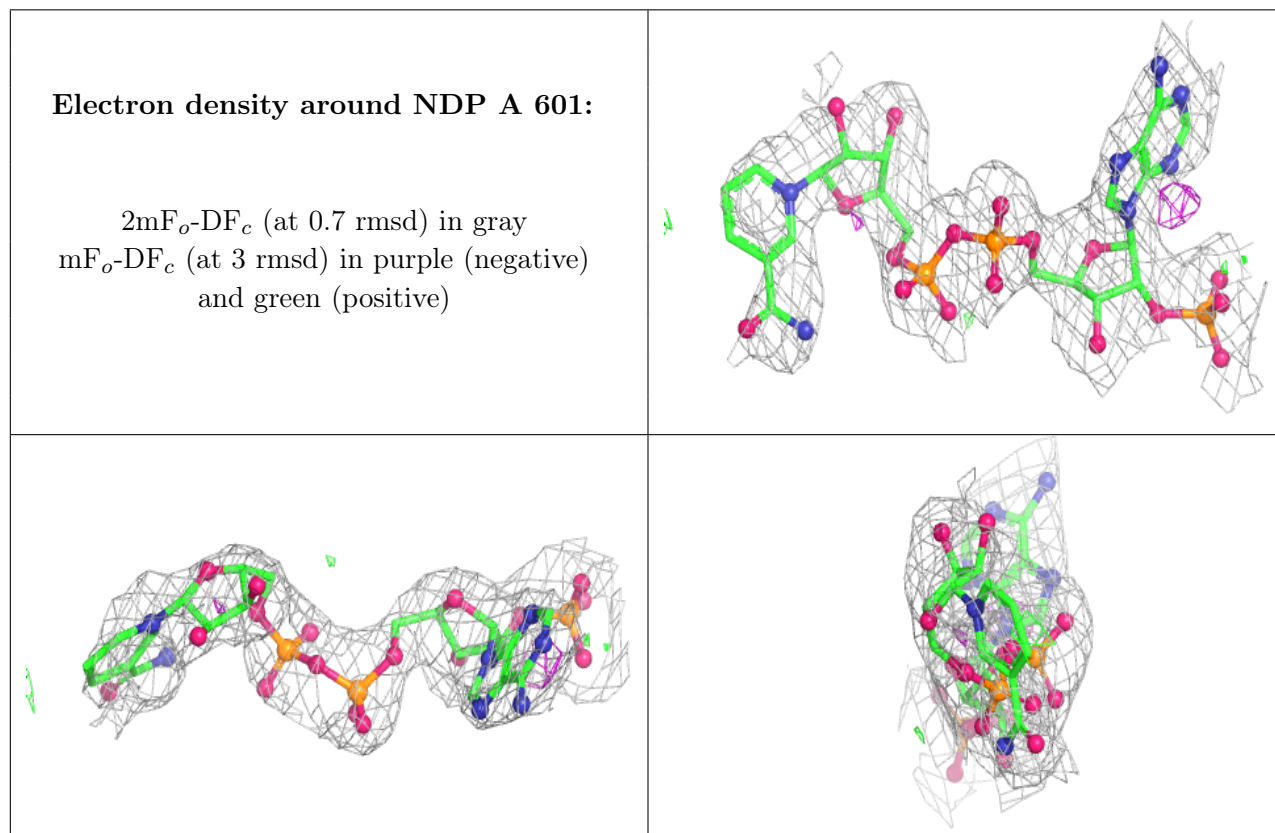
6.3 Carbohydrates [i](#)

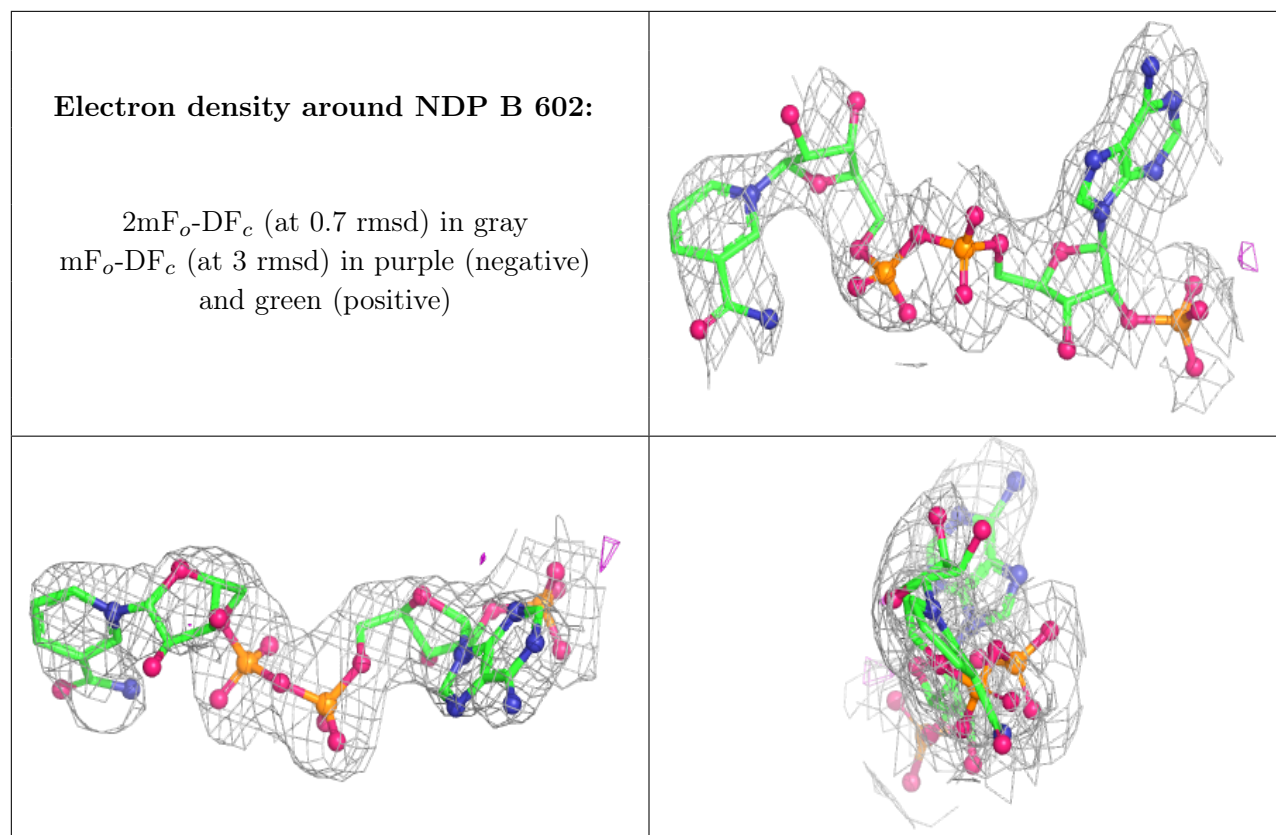
Unable to reproduce the depositors R factor - this section is therefore empty.

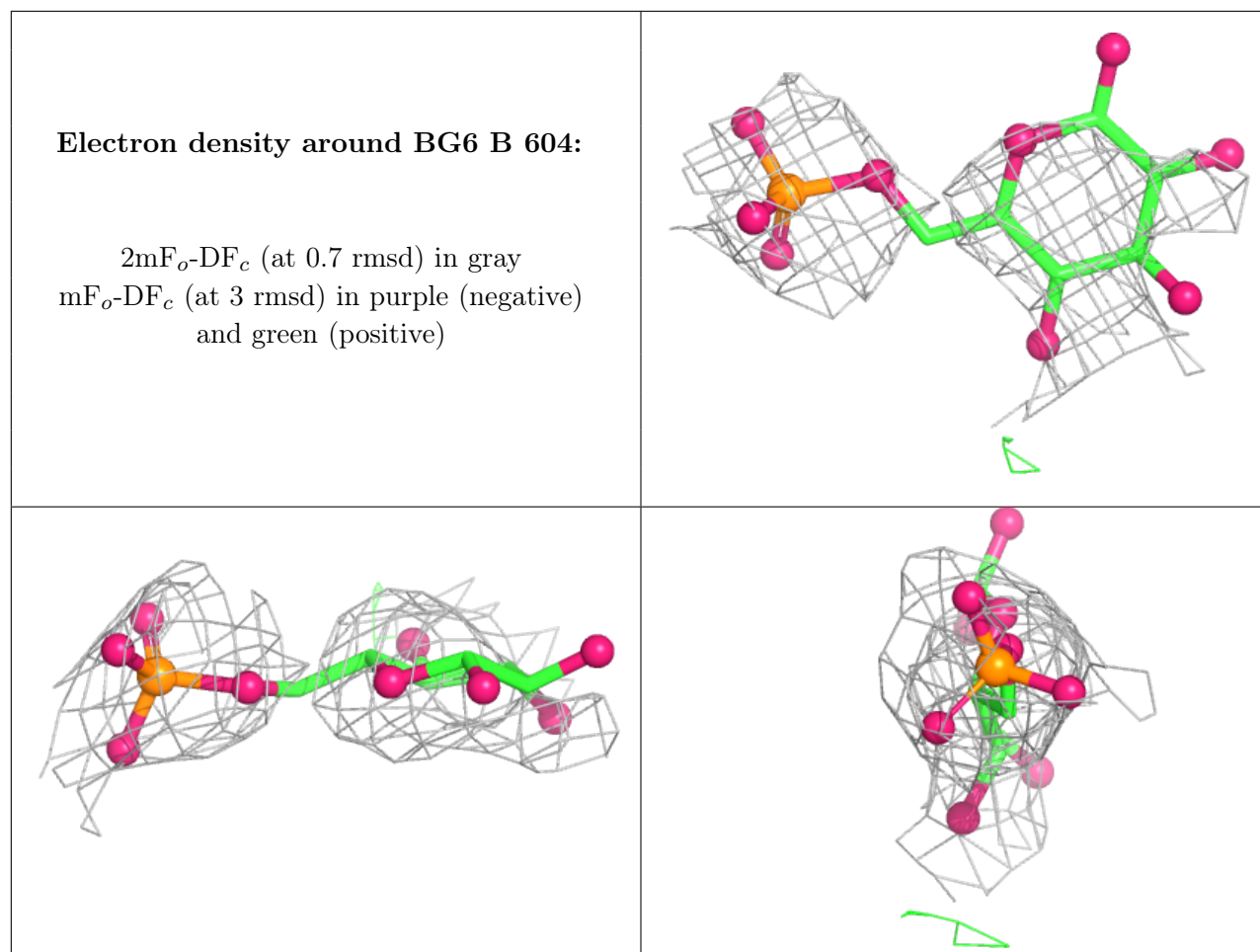
6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.







6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.