Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:32 PM BST

PDB ID	:	6D24
Title	:	Trypanosoma cruzi Glucose-6-P Dehydrogenase in complex with G6P
Authors	:	Botti, H.; Ortiz, C.; Comini, M.A.; Larrieux, N.; Buschiazzo, A.
Deposited on	:	2018-04-12
Resolution	:	3.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

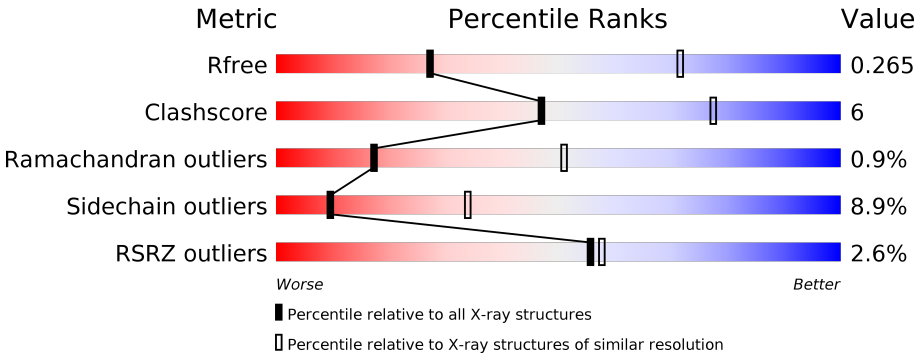
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 on 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	541	4% 72% 19% • 7%
1	B	541	2% 72% 20% • 7%
2	C	541	2% 70% 19% • 9%
2	D	541	% 71% 19% • 9%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	607	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16004 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
1	A	502	Total	C	N	O	S	0	2	0
			3920	2485	684	734	17			
1	B	502	Total	C	N	O	S	0	2	0
			3960	2503	704	737	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP Q1WBU6
A	16	GLY	-	expression tag	UNP Q1WBU6
A	17	SER	-	expression tag	UNP Q1WBU6
A	18	SER	-	expression tag	UNP Q1WBU6
A	19	HIS	-	expression tag	UNP Q1WBU6
A	20	HIS	-	expression tag	UNP Q1WBU6
A	21	HIS	-	expression tag	UNP Q1WBU6
A	22	HIS	-	expression tag	UNP Q1WBU6
A	23	HIS	-	expression tag	UNP Q1WBU6
A	24	HIS	-	expression tag	UNP Q1WBU6
A	25	SER	-	expression tag	UNP Q1WBU6
A	26	SER	-	expression tag	UNP Q1WBU6
A	27	GLY	-	expression tag	UNP Q1WBU6
A	28	LEU	-	expression tag	UNP Q1WBU6
A	29	VAL	-	expression tag	UNP Q1WBU6
A	30	PRO	-	expression tag	UNP Q1WBU6
A	31	ARG	-	expression tag	UNP Q1WBU6
A	32	GLY	-	expression tag	UNP Q1WBU6
A	33	SER	-	expression tag	UNP Q1WBU6
A	34	HIS	-	expression tag	UNP Q1WBU6
A	35	MET	-	expression tag	UNP Q1WBU6
A	36	ALA	-	expression tag	UNP Q1WBU6
A	37	SER	-	expression tag	UNP Q1WBU6
A	290	GLU	ALA	engineered mutation	UNP Q1WBU6
B	15	MET	-	expression tag	UNP Q1WBU6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	GLY	-	expression tag	UNP Q1WBU6
B	17	SER	-	expression tag	UNP Q1WBU6
B	18	SER	-	expression tag	UNP Q1WBU6
B	19	HIS	-	expression tag	UNP Q1WBU6
B	20	HIS	-	expression tag	UNP Q1WBU6
B	21	HIS	-	expression tag	UNP Q1WBU6
B	22	HIS	-	expression tag	UNP Q1WBU6
B	23	HIS	-	expression tag	UNP Q1WBU6
B	24	HIS	-	expression tag	UNP Q1WBU6
B	25	SER	-	expression tag	UNP Q1WBU6
B	26	SER	-	expression tag	UNP Q1WBU6
B	27	GLY	-	expression tag	UNP Q1WBU6
B	28	LEU	-	expression tag	UNP Q1WBU6
B	29	VAL	-	expression tag	UNP Q1WBU6
B	30	PRO	-	expression tag	UNP Q1WBU6
B	31	ARG	-	expression tag	UNP Q1WBU6
B	32	GLY	-	expression tag	UNP Q1WBU6
B	33	SER	-	expression tag	UNP Q1WBU6
B	34	HIS	-	expression tag	UNP Q1WBU6
B	35	MET	-	expression tag	UNP Q1WBU6
B	36	ALA	-	expression tag	UNP Q1WBU6
B	37	SER	-	expression tag	UNP Q1WBU6
B	290	GLU	ALA	engineered mutation	UNP Q1WBU6

- Molecule 2 is a protein called Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	494	Total	C	N	O	S	0	1	0
			3910	2474	694	726	16			
2	D	494	Total	C	N	O	S	0	1	0
			3911	2475	689	731	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	MET	-	expression tag	UNP Q1WBU6
C	16	GLY	-	expression tag	UNP Q1WBU6
C	17	SER	-	expression tag	UNP Q1WBU6
C	18	SER	-	expression tag	UNP Q1WBU6
C	19	HIS	-	expression tag	UNP Q1WBU6
C	20	HIS	-	expression tag	UNP Q1WBU6
C	21	HIS	-	expression tag	UNP Q1WBU6

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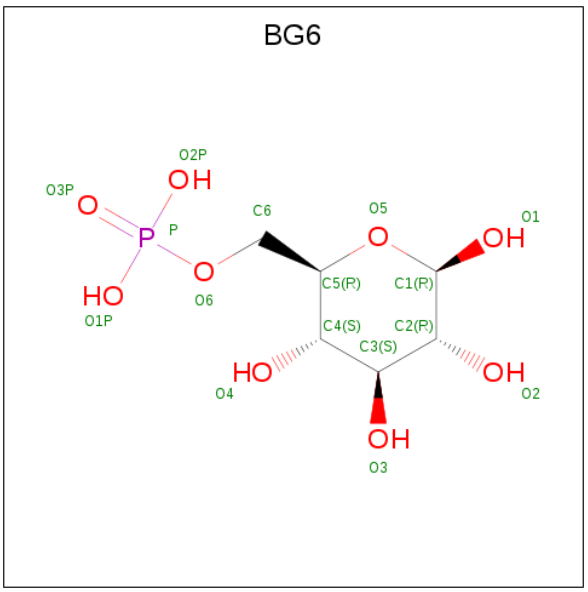
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	HIS	-	expression tag	UNP Q1WBU6
C	23	HIS	-	expression tag	UNP Q1WBU6
C	24	HIS	-	expression tag	UNP Q1WBU6
C	25	SER	-	expression tag	UNP Q1WBU6
C	26	SER	-	expression tag	UNP Q1WBU6
C	27	GLY	-	expression tag	UNP Q1WBU6
C	28	LEU	-	expression tag	UNP Q1WBU6
C	29	VAL	-	expression tag	UNP Q1WBU6
C	30	PRO	-	expression tag	UNP Q1WBU6
C	31	ARG	-	expression tag	UNP Q1WBU6
C	32	GLY	-	expression tag	UNP Q1WBU6
C	33	SER	-	expression tag	UNP Q1WBU6
C	34	HIS	-	expression tag	UNP Q1WBU6
C	35	MET	-	expression tag	UNP Q1WBU6
C	36	ALA	-	expression tag	UNP Q1WBU6
C	37	SER	-	expression tag	UNP Q1WBU6
C	290	GLU	ALA	engineered mutation	UNP Q1WBU6
D	15	MET	-	expression tag	UNP Q1WBU6
D	16	GLY	-	expression tag	UNP Q1WBU6
D	17	SER	-	expression tag	UNP Q1WBU6
D	18	SER	-	expression tag	UNP Q1WBU6
D	19	HIS	-	expression tag	UNP Q1WBU6
D	20	HIS	-	expression tag	UNP Q1WBU6
D	21	HIS	-	expression tag	UNP Q1WBU6
D	22	HIS	-	expression tag	UNP Q1WBU6
D	23	HIS	-	expression tag	UNP Q1WBU6
D	24	HIS	-	expression tag	UNP Q1WBU6
D	25	SER	-	expression tag	UNP Q1WBU6
D	26	SER	-	expression tag	UNP Q1WBU6
D	27	GLY	-	expression tag	UNP Q1WBU6
D	28	LEU	-	expression tag	UNP Q1WBU6
D	29	VAL	-	expression tag	UNP Q1WBU6
D	30	PRO	-	expression tag	UNP Q1WBU6
D	31	ARG	-	expression tag	UNP Q1WBU6
D	32	GLY	-	expression tag	UNP Q1WBU6
D	33	SER	-	expression tag	UNP Q1WBU6
D	34	HIS	-	expression tag	UNP Q1WBU6
D	35	MET	-	expression tag	UNP Q1WBU6
D	36	ALA	-	expression tag	UNP Q1WBU6
D	37	SER	-	expression tag	UNP Q1WBU6
D	290	GLU	ALA	engineered mutation	UNP Q1WBU6

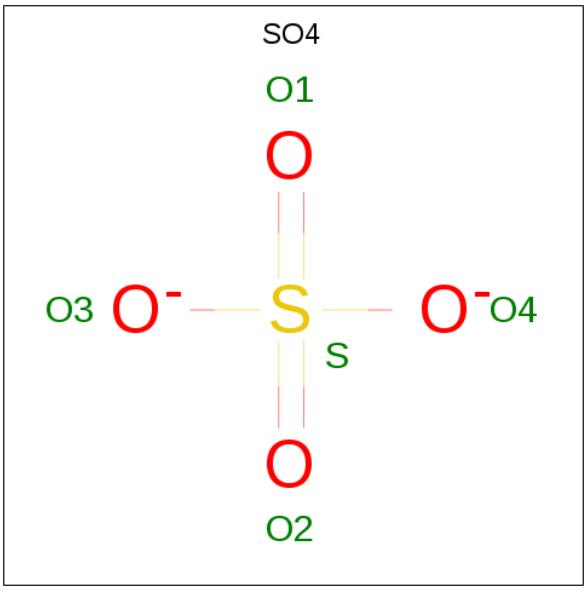
- Molecule 3 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula:

$C_6H_{13}O_9P$).



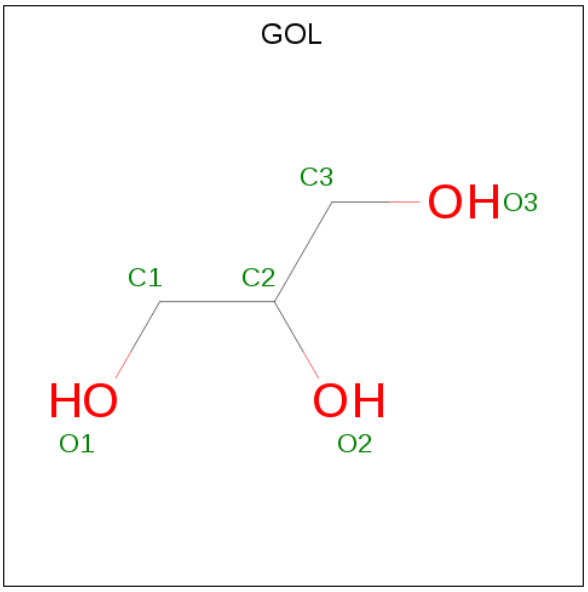
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- 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	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	6	Total Cl 6 6	0	0
6	A	3	Total Cl 3 3	0	0
6	D	8	Total Cl 8 8	0	0
6	C	6	Total Cl 6 6	0	0

- Molecule 7 is water.

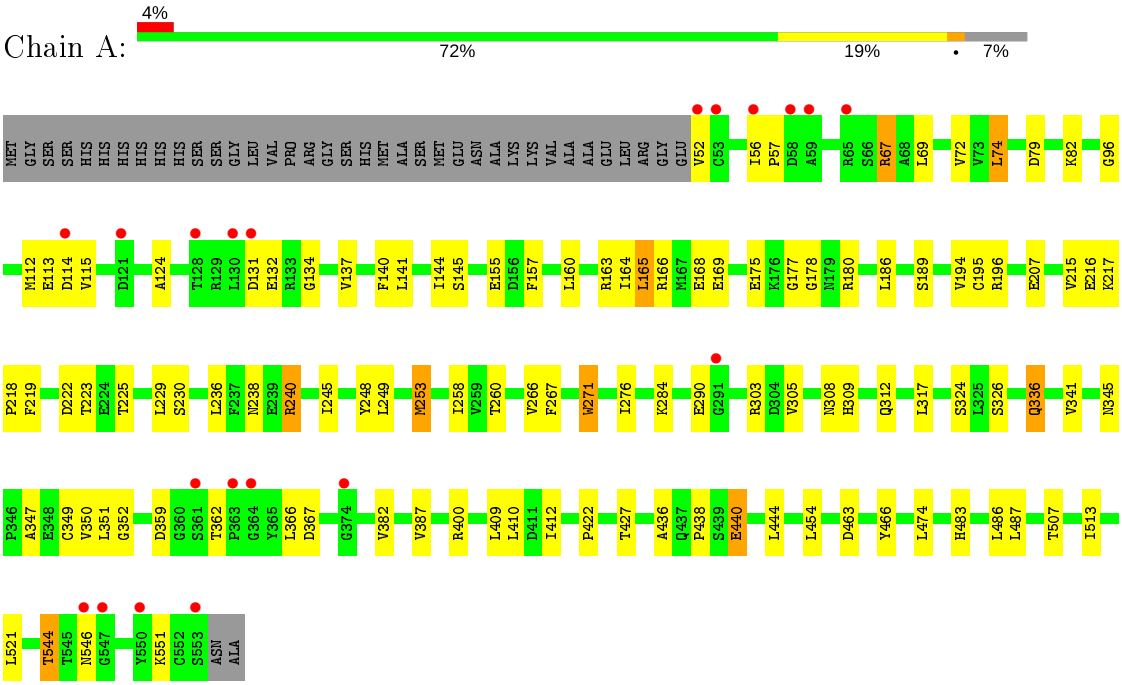
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	8	Total O 8 8	0	0
7	B	9	Total O 9 9	0	0
7	C	17	Total O 17 17	0	0
7	D	13	Total O 13 13	0	0

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.

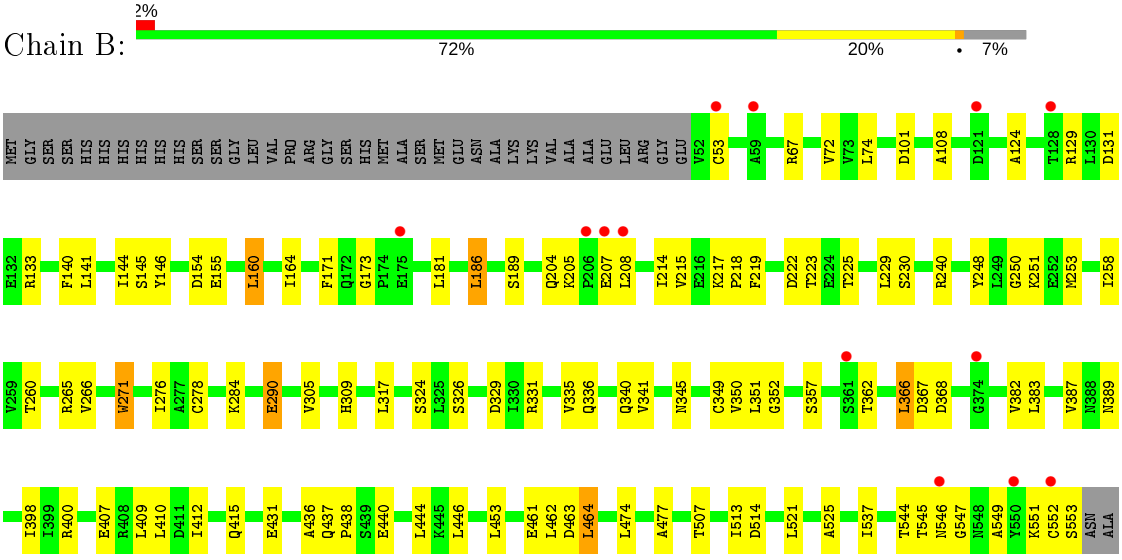
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain A:



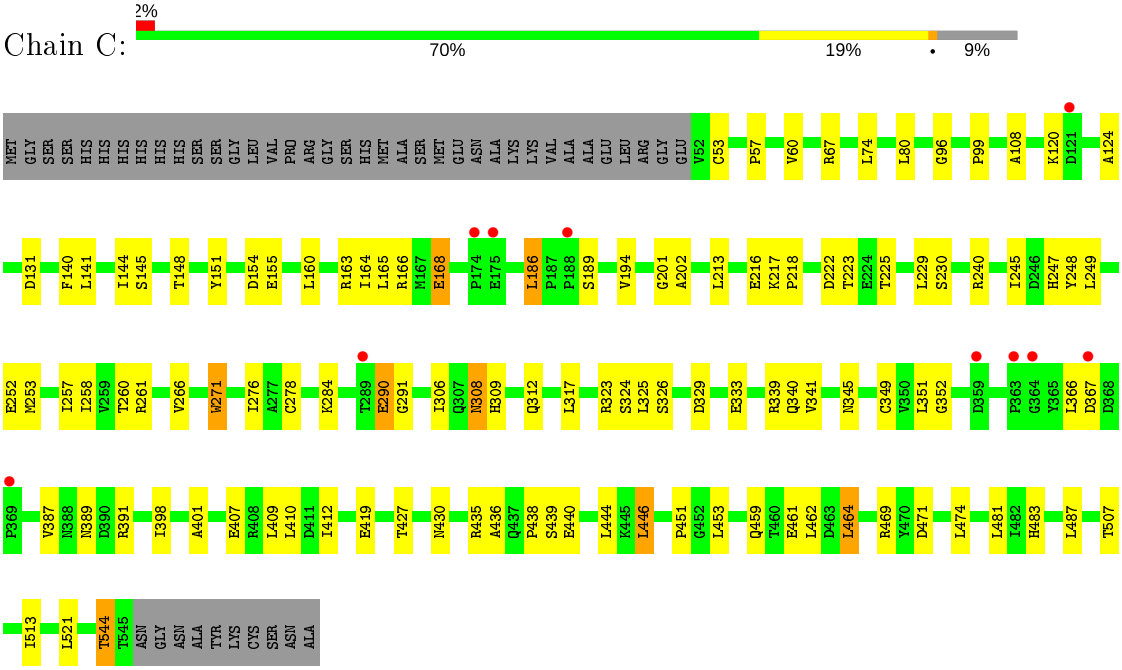
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain B:



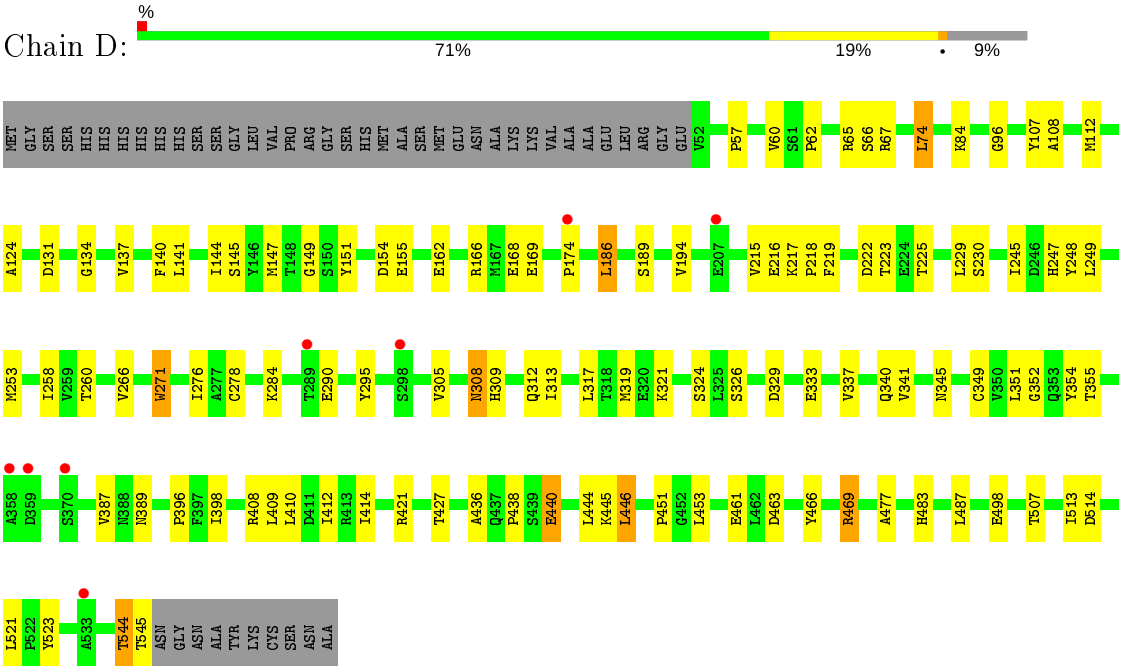
• Molecule 2: Glucose-6-phosphate 1-dehydrogenase

Chain C:



• Molecule 2: Glucose-6-phosphate 1-dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.79Å 133.03Å 107.75Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	34.16 – 3.35 34.07 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.16-3.35) 99.4 (34.07-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.205 , 0.254 0.219 , 0.265	Depositor DCC
R_{free} test set	796 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	16004	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 26.87 % 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 2.4373e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, CSO, SO4, BG6, CL

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	0.52	0/4002	0.74	0/5432
1	B	0.52	0/4041	0.74	0/5477
2	C	0.51	0/3983	0.73	0/5397
2	D	0.51	0/3984	0.73	0/5398
All	All	0.52	0/16010	0.74	0/21704

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3920	0	3833	57	0
1	B	3960	0	3905	44	0
2	C	3910	0	3872	51	0
2	D	3911	0	3872	60	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	1	0
3	D	16	0	11	0	0
4	A	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	25	0	0	0	0
4	C	15	0	0	0	0
4	D	20	0	0	0	0
5	A	18	0	24	4	0
5	B	6	0	8	0	0
5	C	36	0	48	1	0
5	D	24	0	32	1	0
6	A	3	0	0	0	0
6	B	6	0	0	0	0
6	C	6	0	0	1	0
6	D	8	0	0	3	0
7	A	8	0	0	0	0
7	B	9	0	0	0	0
7	C	17	0	0	0	0
7	D	13	0	0	0	0
All	All	16004	0	15638	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (196) 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)
2:D:319:MET:HA	2:D:337:VAL:HG11	1.39	1.05
1:A:238:ASN:HB3	1:A:240:ARG:HE	1.40	0.85
2:D:396:PRO:HB3	6:D:612:CL:CL	2.14	0.84
1:A:382:VAL:HG12	1:A:400:ARG:HG2	1.60	0.82
1:A:218:PRO:HB3	5:A:607:GOL:H11	1.65	0.78
1:A:112:MET:HG2	1:A:115:VAL:HG22	1.72	0.72
1:A:410:LEU:HD23	1:A:436:ALA:HB3	1.71	0.71
2:D:62:PRO:HA	2:D:65:ARG:HG3	1.70	0.71
2:D:410:LEU:HD23	2:D:436:ALA:HB3	1.75	0.69
1:A:196:ARG:HG3	1:A:236:LEU:HD21	1.74	0.68
2:C:410:LEU:HD23	2:C:436:ALA:HB3	1.77	0.67
2:D:62:PRO:HA	2:D:65:ARG:CG	2.25	0.66
2:C:164:ILE:O	2:C:168:GLU:HG2	1.95	0.66
2:D:215:VAL:HG12	2:D:219:PHE:HE1	1.60	0.66
1:A:215:VAL:HG12	1:A:219:PHE:HE1	1.61	0.64
1:A:345:ASN:HD21	1:A:347:ALA:HB3	1.61	0.63
1:B:410:LEU:HD23	1:B:436:ALA:HB3	1.79	0.63
1:B:462:LEU:HD23	2:C:464:LEU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:MET:HA	2:D:337:VAL:CG1	2.25	0.61
2:D:249:LEU:HD11	2:D:312:GLN:NE2	2.17	0.60
1:B:217:LYS:HG2	1:B:218:PRO:HA	1.83	0.60
1:A:249:LEU:HD11	1:A:312:GLN:NE2	2.18	0.58
2:D:60:VAL:O	2:D:65:ARG:HD3	2.04	0.57
1:B:74:LEU:HB3	1:B:186:LEU:HD23	1.85	0.57
1:A:466:TYR:HE2	2:D:451:PRO:HB3	1.68	0.57
1:B:266:VAL:HG21	2:C:444:LEU:HD11	1.87	0.56
2:C:120:LYS:O	2:C:124:ALA:HB3	2.05	0.56
1:A:382:VAL:CG1	1:A:400:ARG:HG2	2.32	0.56
2:D:249:LEU:HD21	2:D:312:GLN:HG3	1.86	0.56
1:A:466:TYR:CE2	2:D:451:PRO:HB3	2.41	0.56
1:A:248:TYR:CD2	1:A:309:HIS:HB3	2.41	0.55
1:B:171:PHE:CZ	1:B:173:GLY:HA3	2.41	0.55
1:A:195:CYS:HB3	1:A:236:LEU:HD23	1.90	0.53
1:B:464:LEU:HB3	2:C:462:LEU:HD23	1.90	0.53
1:A:336:GLN:HG3	2:C:323:ARG:HD3	1.90	0.53
2:D:308:ASN:HD22	2:D:309:HIS:H	1.56	0.53
1:B:205:LYS:HB2	1:B:208:LEU:HD12	1.91	0.52
2:C:217:LYS:HB2	2:C:218:PRO:HA	1.91	0.52
2:D:308:ASN:ND2	2:D:309:HIS:H	2.08	0.51
2:D:217:LYS:HB2	2:D:218:PRO:HA	1.92	0.51
2:D:317:LEU:HD22	2:D:414:ILE:HD11	1.91	0.51
1:A:483:HIS:CE1	1:A:487:LEU:HD11	2.46	0.51
2:D:57:PRO:O	2:D:96:GLY:HA3	2.11	0.51
1:A:284:LYS:HB2	1:A:409:LEU:HB3	1.92	0.51
1:B:284:LYS:HB2	1:B:409:LEU:HB3	1.93	0.51
1:B:265:ARG:HE	2:C:419:GLU:HG2	1.76	0.51
2:D:469:ARG:HD3	6:D:601:CL:CL	2.47	0.50
2:D:134:GLY:O	2:D:137:VAL:HG12	2.11	0.50
2:D:84:LYS:HE3	5:D:610:GOL:H12	1.93	0.50
1:B:341:VAL:HG22	1:B:387:VAL:HG22	1.92	0.50
2:D:305:VAL:HG22	2:D:309:HIS:HD2	1.77	0.50
2:C:247:HIS:HE1	3:C:602:BG6:O5	1.94	0.50
2:C:249:LEU:HD21	2:C:312:GLN:HG3	1.94	0.49
2:C:284:LYS:HB2	2:C:409:LEU:HB3	1.94	0.49
2:D:284:LYS:HB2	2:D:409:LEU:HB3	1.94	0.49
2:D:408:ARG:NH1	6:D:615:CL:CL	2.83	0.49
2:D:151:TYR:HB3	2:D:194:VAL:CG2	2.42	0.49
1:A:238:ASN:HB3	1:A:240:ARG:NE	2.19	0.49
2:D:141:LEU:HD23	2:D:144:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:GLU:O	2:D:166:ARG:HG2	2.13	0.48
1:B:250:GLY:O	1:B:477:ALA:HA	2.13	0.48
2:D:271:TRP:HA	2:D:276:ILE:HD11	1.96	0.48
2:C:247:HIS:HA	2:C:481:LEU:HD11	1.94	0.48
2:D:305:VAL:HA	2:D:308:ASN:HD21	1.78	0.48
1:A:217:LYS:HB2	1:A:218:PRO:HA	1.96	0.48
1:B:271:TRP:HA	1:B:276:ILE:HD11	1.96	0.48
1:B:400:ARG:HH11	1:B:537:ILE:HD13	1.78	0.48
2:C:141:LEU:HD23	2:C:144:ILE:HD12	1.95	0.48
2:C:271:TRP:HA	2:C:276:ILE:HD11	1.96	0.48
1:A:141:LEU:HD23	1:A:144:ILE:HD12	1.96	0.47
1:A:341:VAL:HG22	1:A:387:VAL:HG22	1.96	0.47
2:D:140:PHE:CE2	2:D:144:ILE:HD11	2.49	0.47
1:B:444:LEU:HD11	2:C:266:VAL:HG21	1.95	0.47
1:B:351:LEU:HD11	1:B:513:ILE:HG12	1.96	0.47
2:C:163:ARG:HA	2:C:166:ARG:HH21	1.78	0.47
2:C:223:THR:HG22	2:C:507:THR:HG21	1.95	0.47
1:B:248:TYR:CD2	1:B:309:HIS:HB3	2.49	0.47
2:C:483:HIS:CE1	2:C:487:LEU:HD11	2.49	0.47
1:A:271:TRP:HA	1:A:276:ILE:HD11	1.97	0.47
2:C:57:PRO:O	2:C:96:GLY:HA3	2.14	0.47
1:A:253:MET:HE3	1:A:440:GLU:HB3	1.97	0.47
1:B:415:GLN:HG3	1:B:431:GLU:HB3	1.95	0.47
1:A:350:VAL:HB	1:A:382:VAL:HG22	1.97	0.46
2:C:140:PHE:CE2	2:C:144:ILE:HD11	2.50	0.46
1:B:72:VAL:HG21	1:B:164:ILE:HD11	1.97	0.46
1:A:303:ARG:O	5:A:607:GOL:H2	2.16	0.46
1:A:444:LEU:HD11	2:D:266:VAL:HG21	1.96	0.46
2:C:257:ILE:O	2:C:261:ARG:HG2	2.16	0.46
2:D:351:LEU:HD11	2:D:513:ILE:HG12	1.96	0.46
1:A:157:PHE:HE1	1:A:194:VAL:HG13	1.80	0.46
1:A:57:PRO:O	1:A:96:GLY:HA3	2.15	0.46
1:B:108:ALA:HB3	1:B:146:TYR:OH	2.16	0.46
1:A:56:ILE:HG13	1:A:56:ILE:O	2.16	0.46
2:C:341:VAL:HG22	2:C:387:VAL:HG22	1.98	0.46
1:B:340:GLN:OE1	1:B:389:ASN:HB3	2.16	0.46
2:D:108:ALA:HA	2:D:151:TYR:OH	2.16	0.46
1:B:547:GLY:HA2	1:B:553:SER:HA	1.98	0.46
1:B:140:PHE:CE2	1:B:144:ILE:HD11	2.51	0.45
1:A:140:PHE:CE2	1:A:144:ILE:HD11	2.50	0.45
1:B:331:ARG:O	1:B:335:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HD3	1:B:133:ARG:HH21	1.81	0.45
2:C:248:TYR:CD2	2:C:309:HIS:HB3	2.51	0.45
2:D:223:THR:HG22	2:D:507:THR:HG21	1.97	0.45
1:A:352:GLY:HA2	1:A:521:LEU:O	2.17	0.45
1:B:317:LEU:HD21	1:B:412:ILE:HG21	1.99	0.45
2:D:151:TYR:HB3	2:D:194:VAL:HG22	1.99	0.45
1:A:267:PHE:CE2	2:D:446:LEU:HD11	2.51	0.45
1:B:141:LEU:HD23	1:B:144:ILE:HD12	1.98	0.45
2:C:351:LEU:HD11	2:C:513:ILE:HG12	1.99	0.45
2:D:483:HIS:CE1	2:D:487:LEU:HD11	2.51	0.45
2:C:340:GLN:HG2	2:D:421:ARG:CZ	2.47	0.45
1:B:223:THR:HG22	1:B:507:THR:HG21	1.99	0.45
2:C:464:LEU:HD12	2:C:469:ARG:HG3	1.98	0.45
2:C:80:LEU:HB2	5:C:607:GOL:H2	1.99	0.44
2:D:341:VAL:HG22	2:D:387:VAL:HG22	1.99	0.44
2:D:248:TYR:CG	2:D:309:HIS:HB3	2.52	0.44
2:C:324:SER:HB3	2:C:329:ASP:OD2	2.16	0.44
2:C:352:GLY:HA2	2:C:521:LEU:O	2.17	0.44
1:A:351:LEU:HD11	1:A:513:ILE:HG12	1.99	0.44
2:C:160:LEU:HG	2:C:164:ILE:HD11	2.00	0.44
2:D:340:GLN:HE22	2:D:389:ASN:HD22	1.66	0.44
1:A:67:ARG:HG2	1:A:178:GLY:N	2.33	0.43
2:D:445:LYS:NZ	2:D:545:THR:HG21	2.32	0.43
1:A:134:GLY:O	1:A:137:VAL:HG12	2.18	0.43
1:A:267:PHE:HE2	2:D:446:LEU:HD21	1.82	0.43
2:D:352:GLY:HA2	2:D:521:LEU:O	2.19	0.43
1:A:113:GLU:HG2	1:A:114:ASP:N	2.33	0.43
2:D:324:SER:HB3	2:D:329:ASP:OD2	2.18	0.43
2:C:108:ALA:O	2:C:148:THR:HA	2.19	0.43
2:D:107:TYR:HA	2:D:147:MET:O	2.19	0.43
1:A:266:VAL:HG21	2:D:444:LEU:HD11	2.01	0.43
1:B:357:SER:HB3	1:B:525:ALA:O	2.19	0.43
2:D:248:TYR:CD2	2:D:309:HIS:HB3	2.53	0.43
1:A:72:VAL:HG21	1:A:164:ILE:HD11	2.01	0.43
1:A:544:THR:HG22	1:A:546:ASN:H	1.83	0.43
2:C:391:ARG:NH2	6:C:615:CL:CL	2.89	0.43
2:C:435:ARG:HH21	2:C:439:SER:HB3	1.83	0.43
2:D:107:TYR:CZ	2:D:149:GLY:HA3	2.54	0.43
1:A:165:LEU:HA	1:A:168:GLU:HB2	2.01	0.43
1:A:223:THR:HG22	1:A:507:THR:HG21	2.00	0.43
2:C:308:ASN:ND2	2:C:309:HIS:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:HG12	1:B:219:PHE:CE1	2.54	0.43
2:C:290:GLU:HB3	2:C:291:GLY:H	1.74	0.43
2:C:430:ASN:HD22	2:C:446:LEU:HA	1.84	0.43
2:D:107:TYR:HD2	2:D:147:MET:SD	2.42	0.43
2:D:354:TYR:HA	2:D:523:TYR:O	2.19	0.43
1:B:324:SER:HB3	1:B:329:ASP:OD2	2.19	0.42
1:A:317:LEU:HD21	1:A:412:ILE:HG21	2.01	0.42
1:B:350:VAL:HB	1:B:382:VAL:HG22	2.01	0.42
1:B:72:VAL:HG12	1:B:74:LEU:HD22	2.02	0.42
2:C:317:LEU:HD21	2:C:412:ILE:HG21	2.02	0.42
2:D:124:ALA:HB2	2:D:141:LEU:HD11	2.02	0.42
1:A:124:ALA:HB2	1:A:141:LEU:HD11	2.01	0.42
1:B:352:GLY:HA2	1:B:521:LEU:O	2.20	0.42
2:C:340:GLN:HE22	2:C:389:ASN:HD22	1.66	0.42
1:B:181:LEU:HD11	1:B:214:ILE:HD12	2.01	0.42
1:A:67:ARG:CZ	1:A:175:GLU:HG2	2.50	0.42
1:A:112:MET:HG2	1:A:115:VAL:CG2	2.47	0.42
1:A:164:ILE:HD13	1:A:180:ARG:HD3	2.02	0.42
1:A:218:PRO:CB	5:A:607:GOL:H11	2.44	0.42
2:D:317:LEU:HD21	2:D:412:ILE:HG21	2.02	0.41
1:A:218:PRO:HB3	5:A:607:GOL:C1	2.44	0.41
2:C:151:TYR:HB3	2:C:194:VAL:CG2	2.50	0.41
2:D:278:CYS:SG	2:D:398:ILE:HD12	2.60	0.41
1:A:74:LEU:HD22	1:A:194:VAL:HG11	2.02	0.41
2:D:74:LEU:HB3	2:D:186:LEU:HD23	2.02	0.41
1:A:474:LEU:HD21	2:D:451:PRO:HB2	2.03	0.41
2:D:216:GLU:HA	2:D:245:ILE:HG22	2.01	0.41
2:C:60:VAL:HG11	2:C:99:PRO:HA	2.02	0.41
1:A:166:ARG:HH21	1:A:169:GLU:CD	2.24	0.41
1:B:204:GLN:HE21	1:B:208:LEU:HB2	1.85	0.41
1:B:251:LYS:HE2	1:B:437:GLN:OE1	2.19	0.41
1:B:284:LYS:HB3	1:B:407:GLU:O	2.21	0.41
1:B:474:LEU:HD21	2:C:451:PRO:HB2	2.03	0.41
1:B:72:VAL:HG11	1:B:160:LEU:HD11	2.03	0.41
2:C:186:LEU:HD22	2:C:194:VAL:HG21	2.01	0.41
2:C:252:GLU:HG2	2:C:474:LEU:HD13	2.02	0.41
1:A:422:PRO:HD3	2:D:321:LYS:HD3	2.02	0.41
2:D:66:SER:O	2:D:174:PRO:HD2	2.21	0.41
2:C:306:ILE:HD11	2:C:401:ALA:HB3	2.03	0.41
1:A:216:GLU:HA	1:A:245:ILE:HG22	2.03	0.41
1:B:549:ALA:H	1:B:552:CYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:446:LEU:HD21	2:C:462:LEU:CD1	2.51	0.41
2:C:446:LEU:HD21	2:C:462:LEU:HD12	2.03	0.40
1:A:69:LEU:HD21	1:A:486:LEU:HD22	2.04	0.40
2:D:247:HIS:O	2:D:477:ALA:HB1	2.20	0.40
1:A:79:ASP:HA	1:A:82:LYS:HD2	2.02	0.40
2:C:216:GLU:HA	2:C:245:ILE:HG22	2.04	0.40
2:C:325:LEU:HA	2:C:325:LEU:HD23	1.97	0.40
2:C:284:LYS:HB3	2:C:407:GLU:O	2.22	0.40
2:D:440:GLU:O	2:D:466:TYR:HB2	2.21	0.40
1:A:410:LEU:HD23	1:A:436:ALA:CB	2.45	0.40
1:B:124:ALA:HB2	1:B:141:LEU:HD11	2.04	0.40
1:B:366:LEU:C	1:B:368:ASP:H	2.25	0.40
1:B:278:CYS:SG	1:B:398:ILE:HD12	2.62	0.40
2:C:278:CYS:SG	2:C:398:ILE:HD12	2.61	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	502/541 (93%)	464 (92%)	33 (7%)	5 (1%)	15	49
1	B	502/541 (93%)	456 (91%)	40 (8%)	6 (1%)	13	44
2	C	492/541 (91%)	454 (92%)	33 (7%)	5 (1%)	15	49
2	D	492/541 (91%)	459 (93%)	31 (6%)	2 (0%)	34	68
All	All	1988/2164 (92%)	1833 (92%)	137 (7%)	18 (1%)	17	51

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLU

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Mol	Chain	Res	Type
1	A	544	THR
1	B	290	GLU
1	B	544	THR
1	B	546	ASN
2	C	202	ALA
2	C	544	THR
2	D	544	THR
1	B	545	THR
1	A	367	ASP
1	A	438	PRO
1	B	438	PRO
2	C	201	GLY
2	C	367	ASP
2	C	438	PRO
2	D	438	PRO
1	B	367	ASP
1	A	177	GLY

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	414/462 (90%)	378 (91%)	36 (9%)	10 35
1	B	421/462 (91%)	384 (91%)	37 (9%)	10 34
2	C	417/461 (90%)	379 (91%)	38 (9%)	9 33
2	D	419/461 (91%)	381 (91%)	38 (9%)	9 33
All	All	1671/1846 (90%)	1522 (91%)	149 (9%)	9 34

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	67	ARG
1	A	74	LEU
1	A	131	ASP

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	145	SER
1	A	155	GLU
1	A	160	LEU
1	A	163	ARG
1	A	165	LEU
1	A	186	LEU
1	A	189	SER
1	A	207	GLU
1	A	222	ASP
1	A	225	THR
1	A	229	LEU
1	A	230	SER
1	A	240	ARG
1	A	253	MET
1	A	258	ILE
1	A	260	THR
1	A	271	TRP
1	A	305	VAL
1	A	308	ASN
1	A	324	SER
1	A	326	SER
1	A	336	GLN
1	A	349	CYS
1	A	359	ASP
1	A	362	THR
1	A	366	LEU
1	A	427	THR
1	A	440	GLU
1	A	454	LEU
1	A	463	ASP
1	A	551	LYS
1	B	53	CYS
1	B	67	ARG
1	B	101	ASP
1	B	131	ASP
1	B	145	SER
1	B	154	ASP
1	B	155	GLU
1	B	160	LEU
1	B	186	LEU
1	B	189	SER

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Mol	Chain	Res	Type
1	B	207	GLU
1	B	222	ASP
1	B	225	THR
1	B	229	LEU
1	B	230	SER
1	B	240	ARG
1	B	253	MET
1	B	258	ILE
1	B	260	THR
1	B	271	TRP
1	B	290	GLU
1	B	305	VAL
1	B	326	SER
1	B	336	GLN
1	B	345	ASN
1	B	349	CYS
1	B	362	THR
1	B	366	LEU
1	B	383	LEU
1	B	440	GLU
1	B	446	LEU
1	B	453	LEU
1	B	461	GLU
1	B	463	ASP
1	B	464	LEU
1	B	514	ASP
1	B	551	LYS
2	C	53	CYS
2	C	67	ARG
2	C	74	LEU
2	C	131	ASP
2	C	145	SER
2	C	154	ASP
2	C	155	GLU
2	C	165	LEU
2	C	168	GLU
2	C	186	LEU
2	C	189	SER
2	C	213	LEU
2	C	222	ASP
2	C	225	THR
2	C	229	LEU

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Mol	Chain	Res	Type
2	C	230	SER
2	C	240	ARG
2	C	253	MET
2	C	258	ILE
2	C	260	THR
2	C	271	TRP
2	C	290	GLU
2	C	308	ASN
2	C	326	SER
2	C	333	GLU
2	C	339	ARG
2	C	345	ASN
2	C	349	CYS
2	C	366	LEU
2	C	427	THR
2	C	440	GLU
2	C	446	LEU
2	C	453	LEU
2	C	459	GLN
2	C	461	GLU
2	C	464	LEU
2	C	471	ASP
2	C	544	THR
2	D	67	ARG
2	D	74	LEU
2	D	112	MET
2	D	131	ASP
2	D	145	SER
2	D	154	ASP
2	D	155	GLU
2	D	168	GLU
2	D	169	GLU
2	D	186	LEU
2	D	189	SER
2	D	222	ASP
2	D	225	THR
2	D	229	LEU
2	D	230	SER
2	D	253	MET
2	D	258	ILE
2	D	260	THR
2	D	271	TRP

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Mol	Chain	Res	Type
2	D	290	GLU
2	D	295	TYR
2	D	308	ASN
2	D	313	ILE
2	D	326	SER
2	D	333	GLU
2	D	345	ASN
2	D	349	CYS
2	D	355	THR
2	D	427	THR
2	D	440	GLU
2	D	446	LEU
2	D	453	LEU
2	D	461	GLU
2	D	463	ASP
2	D	469	ARG
2	D	498	GLU
2	D	514	ASP
2	D	544	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	139	ASN
1	A	280	GLN
1	A	308	ASN
1	A	340	GLN
1	A	345	ASN
1	B	428	GLN
2	C	91	GLN
2	C	95	ASN
2	C	139	ASN
2	C	247	HIS
2	C	308	ASN
2	C	340	GLN
2	D	91	GLN
2	D	139	ASN
2	D	308	ASN
2	D	340	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSO	C	528	2	3,6,7	0.81	0	0,6,8	0.00	-
2	CSO	D	528	2	3,6,7	0.60	0	0,6,8	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	C	528	2	-	0/1/5/7	-
2	CSO	D	528	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 58 ligands modelled in this entry, 23 are monoatomic - leaving 35 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	BG6	C	602	-	16,16,16	0.52	0	24,24,24	0.61	0
4	SO4	B	605	-	4,4,4	0.09	0	6,6,6	0.29	0
4	SO4	A	605	-	4,4,4	0.19	0	6,6,6	0.17	0
5	GOL	D	608	-	5,5,5	0.24	0	5,5,5	0.28	0
4	SO4	A	602	-	4,4,4	0.23	0	6,6,6	0.17	0
4	SO4	D	604	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	A	606	-	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	D	603	-	4,4,4	0.25	0	6,6,6	0.34	0
5	GOL	C	606	-	5,5,5	0.18	0	5,5,5	0.42	0
5	GOL	C	608	-	5,5,5	0.16	0	5,5,5	0.70	0
5	GOL	D	607	-	5,5,5	0.19	0	5,5,5	0.25	0
3	BG6	A	601	-	16,16,16	0.36	0	24,24,24	0.53	0
4	SO4	B	604	-	4,4,4	0.18	0	6,6,6	0.45	0
5	GOL	A	612	-	5,5,5	0.18	0	5,5,5	0.41	0
4	SO4	B	603	-	4,4,4	0.22	0	6,6,6	0.28	0
5	GOL	C	609	-	5,5,5	0.13	0	5,5,5	0.27	0
4	SO4	C	603	-	4,4,4	0.08	0	6,6,6	0.18	0
5	GOL	D	609	-	5,5,5	0.09	0	5,5,5	0.24	0
4	SO4	B	606	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	C	605	-	4,4,4	0.17	0	6,6,6	0.15	0
3	BG6	D	602	-	16,16,16	0.40	0	24,24,24	0.66	0
5	GOL	A	607	-	5,5,5	0.16	0	5,5,5	0.53	0
5	GOL	D	610	-	5,5,5	0.20	0	5,5,5	0.36	0
4	SO4	B	607	-	4,4,4	0.13	0	6,6,6	0.25	0
4	SO4	C	604	-	4,4,4	0.21	0	6,6,6	0.22	0
3	BG6	B	602	-	16,16,16	0.43	0	24,24,24	0.68	0
5	GOL	C	607	-	5,5,5	0.21	0	5,5,5	0.50	0
5	GOL	A	608	-	5,5,5	0.11	0	5,5,5	0.22	0
4	SO4	D	606	-	4,4,4	0.26	0	6,6,6	0.27	0
5	GOL	B	608	-	5,5,5	0.15	0	5,5,5	0.25	0
5	GOL	C	616	-	5,5,5	0.12	0	5,5,5	0.20	0
5	GOL	C	601	-	5,5,5	0.13	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	604	-	4,4,4	0.10	0	6,6,6	0.24	0
4	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.35	0
4	SO4	D	605	-	4,4,4	0.20	0	6,6,6	0.11	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	BG6	D	602	-	-	2/6/26/26	0/1/1/1
3	BG6	C	602	-	-	3/6/26/26	0/1/1/1
5	GOL	A	608	-	-	0/4/4/4	-
5	GOL	A	607	-	-	0/4/4/4	-
5	GOL	D	607	-	-	0/4/4/4	-
5	GOL	C	606	-	-	0/4/4/4	-
3	BG6	A	601	-	-	2/6/26/26	0/1/1/1
5	GOL	D	608	-	-	0/4/4/4	-
5	GOL	A	612	-	-	1/4/4/4	-
5	GOL	B	608	-	-	0/4/4/4	-
5	GOL	D	610	-	-	3/4/4/4	-
5	GOL	C	609	-	-	2/4/4/4	-
5	GOL	D	609	-	-	0/4/4/4	-
5	GOL	C	601	-	-	0/4/4/4	-
5	GOL	C	608	-	-	0/4/4/4	-
5	GOL	C	616	-	-	2/4/4/4	-
5	GOL	C	607	-	-	0/4/4/4	-
3	BG6	B	602	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	BG6	O5-C5-C6-O6
3	C	602	BG6	C4-C5-C6-O6
3	A	601	BG6	O5-C5-C6-O6
3	A	601	BG6	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	602	BG6	O5-C5-C6-O6
3	D	602	BG6	C4-C5-C6-O6
3	B	602	BG6	O5-C5-C6-O6
3	B	602	BG6	C4-C5-C6-O6
5	D	610	GOL	O1-C1-C2-O2
5	A	612	GOL	C1-C2-C3-O3
5	C	609	GOL	O1-C1-C2-C3
5	D	610	GOL	O1-C1-C2-C3
5	C	616	GOL	O1-C1-C2-C3
5	C	616	GOL	O1-C1-C2-O2
3	C	602	BG6	C6-O6-P-O3P
5	C	609	GOL	O1-C1-C2-O2
5	D	610	GOL	C1-C2-C3-O3

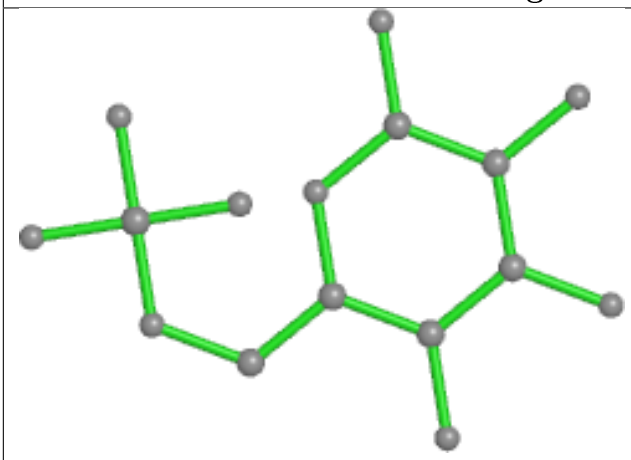
There are no ring outliers.

4 monomers are involved in 7 short contacts:

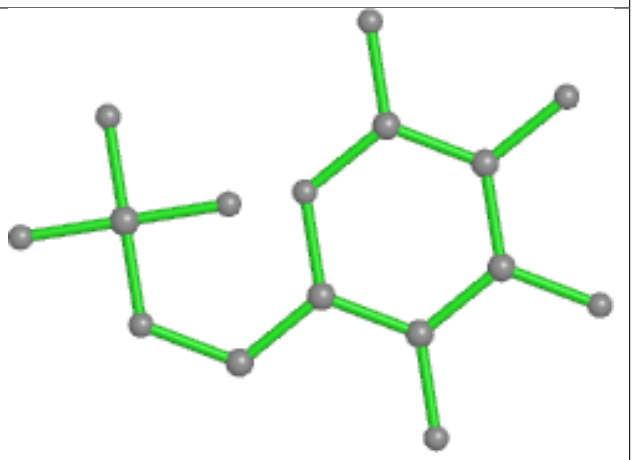
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	BG6	1	0
5	A	607	GOL	4	0
5	D	610	GOL	1	0
5	C	607	GOL	1	0

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 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.

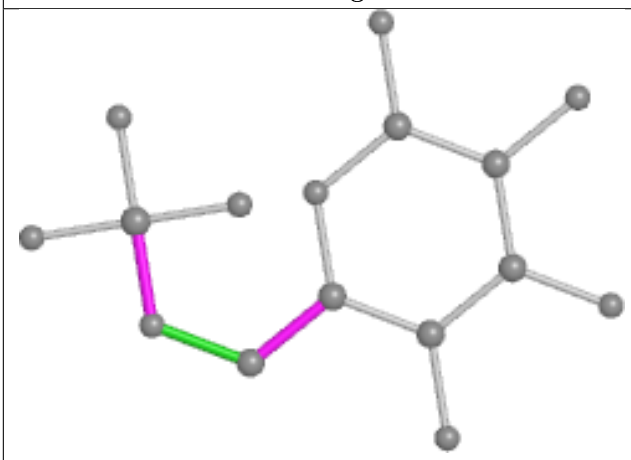
Ligand BG6 C 602



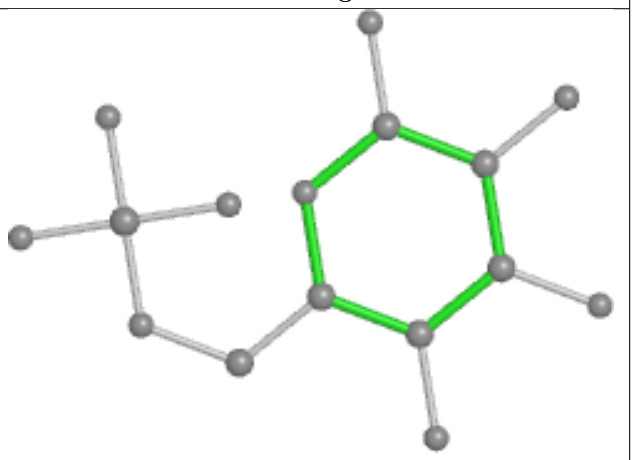
Bond lengths



Bond angles

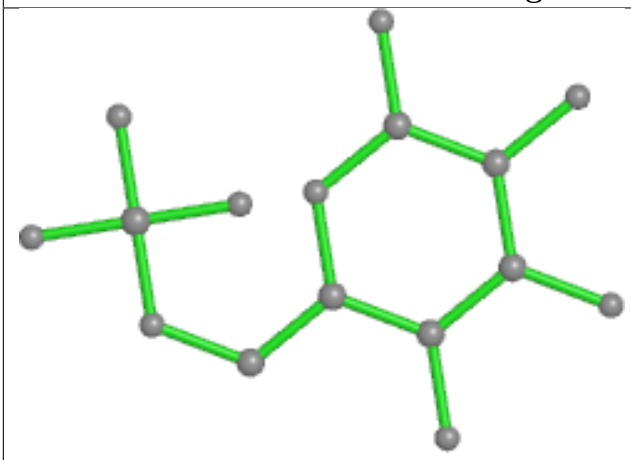


Torsions

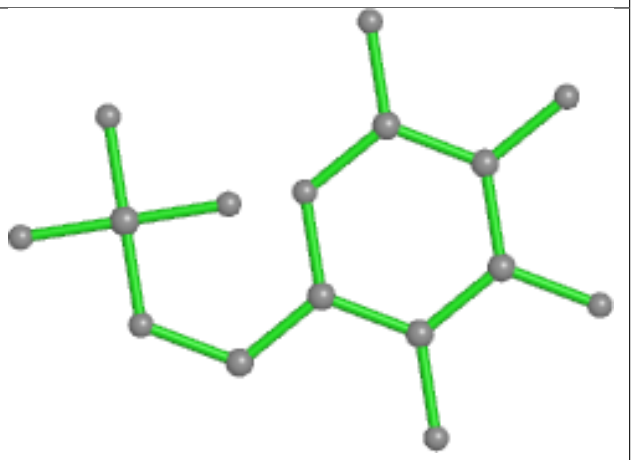


Rings

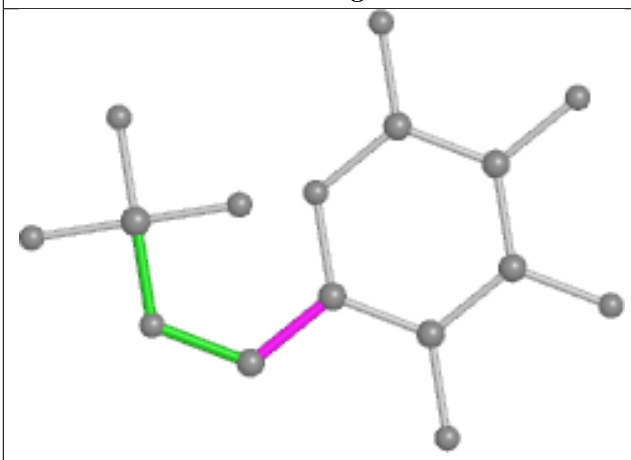
Ligand BG6 A 601



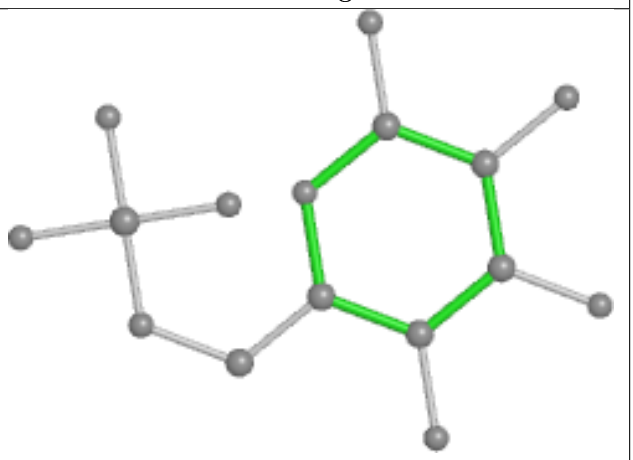
Bond lengths



Bond angles

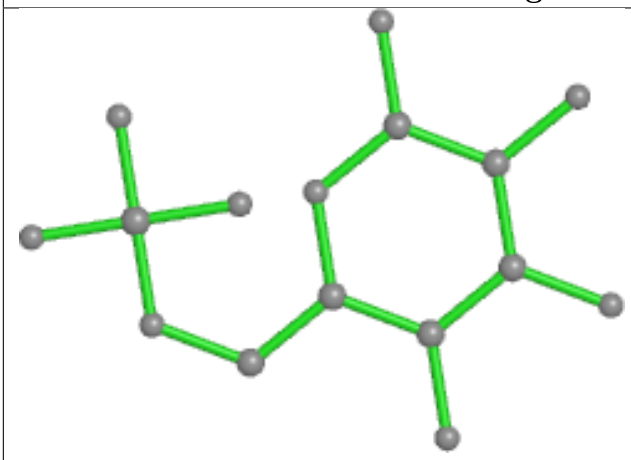


Torsions

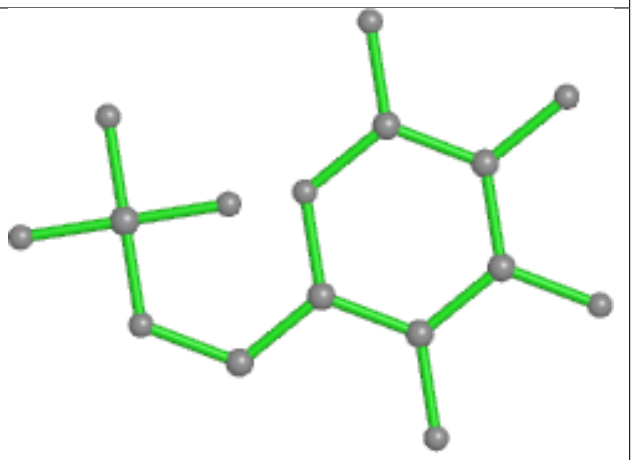


Rings

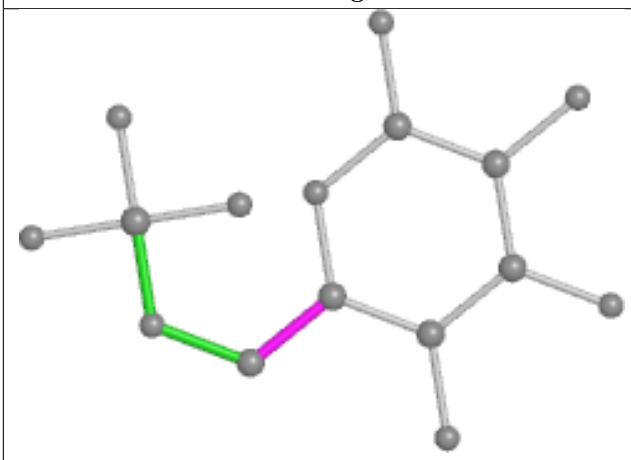
Ligand BG6 D 602



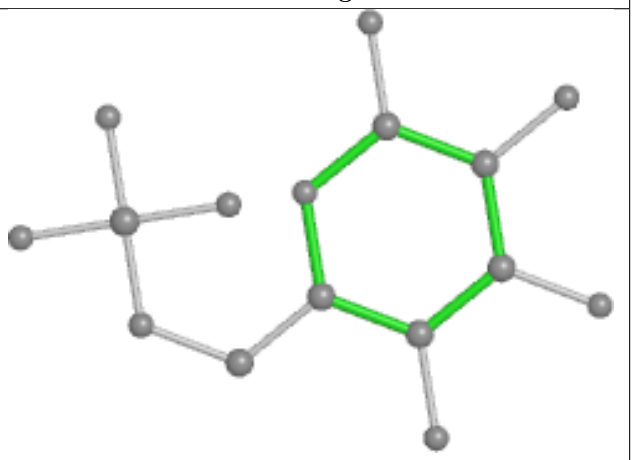
Bond lengths



Bond angles

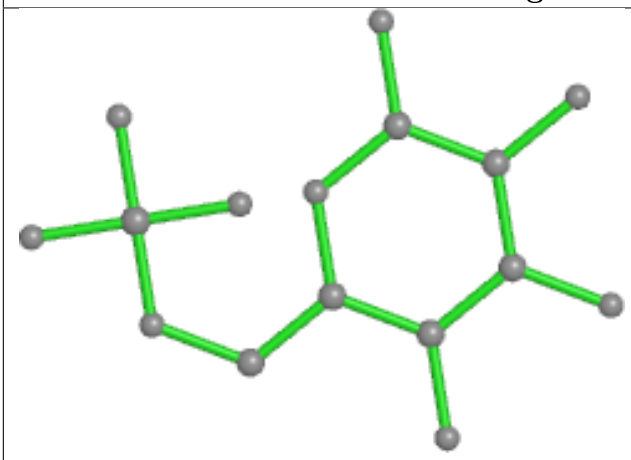


Torsions

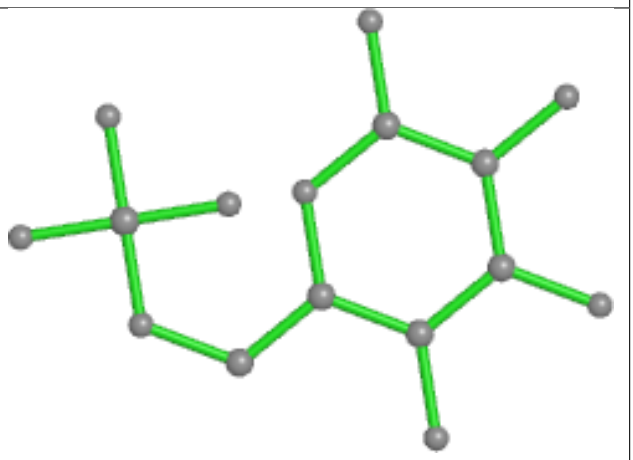


Rings

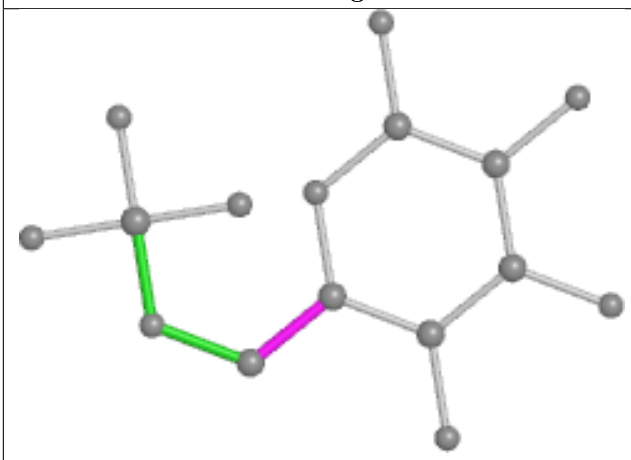
Ligand BG6 B 602



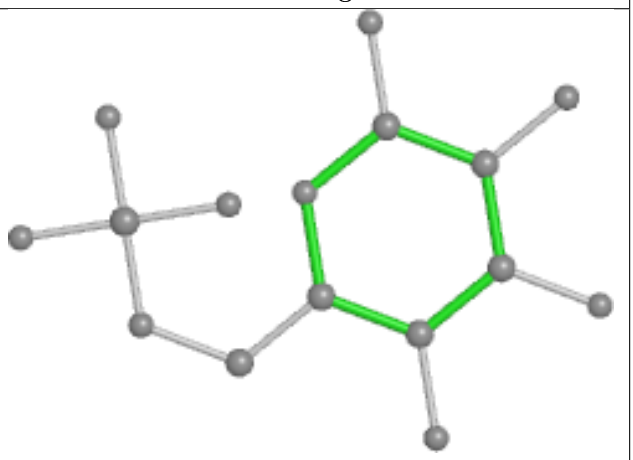
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	502/541 (92%)	-0.02	20 (3%) 38 40	9, 35, 73, 98	0
1	B	502/541 (92%)	-0.09	13 (2%) 56 58	10, 33, 71, 93	0
2	C	493/541 (91%)	-0.08	10 (2%) 65 68	9, 33, 71, 89	0
2	D	493/541 (91%)	-0.13	8 (1%) 72 74	6, 33, 69, 83	0
All	All	1990/2164 (91%)	-0.08	51 (2%) 56 58	6, 33, 71, 98	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	359	ASP	4.3
1	B	128	THR	3.3
1	A	547	GLY	3.3
1	B	374	GLY	3.2
1	A	546	ASN	3.1
1	A	53	CYS	3.1
1	A	374	GLY	3.1
1	B	121	ASP	3.0
1	B	53	CYS	3.0
1	B	207	GLU	2.9
1	B	550	TYR	2.8
2	D	359	ASP	2.8
1	B	552	CYS	2.8
1	B	175	GLU	2.8
1	B	546	ASN	2.7
1	A	114	ASP	2.7
2	C	367	ASP	2.6
1	B	206	PRO	2.6
2	C	369	PRO	2.6
1	A	52	VAL	2.5
1	A	58	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	361	SER	2.5
2	C	175	GLU	2.5
1	A	128	THR	2.5
1	A	65	ARG	2.5
2	D	358	ALA	2.5
2	D	370	SER	2.5
1	B	361	SER	2.4
2	C	364	GLY	2.4
2	D	207	GLU	2.4
2	C	363	PRO	2.4
2	D	298	SER	2.3
2	C	121	ASP	2.3
1	B	59	ALA	2.3
1	A	121	ASP	2.3
2	D	174	PRO	2.3
1	A	130	LEU	2.3
1	A	364	GLY	2.3
2	D	289	THR	2.2
1	B	208	LEU	2.2
2	C	174	PRO	2.2
1	A	550	TYR	2.1
1	A	363	PRO	2.1
1	A	59	ALA	2.1
1	A	56	ILE	2.1
1	A	131	ASP	2.1
2	C	289	THR	2.1
2	D	533	ALA	2.1
1	A	291	GLY	2.1
2	C	188	PRO	2.0
1	A	553	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CSO	D	528	7/8	0.84	0.29	47,49,51,52	0
2	CSO	C	528	7/8	0.89	0.20	38,40,42,43	0

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	D	610	6/6	0.75	0.36	36,40,42,42	0
4	SO4	D	606	5/5	0.76	0.34	82,82,83,85	0
6	CL	C	612	1/1	0.78	0.21	64,64,64,64	0
6	CL	C	614	1/1	0.79	0.20	61,61,61,61	0
6	CL	B	601	1/1	0.80	0.15	59,59,59,59	0
4	SO4	D	604	5/5	0.80	0.35	78,79,80,81	0
4	SO4	C	605	5/5	0.80	0.30	92,92,93,95	0
6	CL	D	614	1/1	0.81	0.21	72,72,72,72	0
6	CL	A	611	1/1	0.81	0.10	48,48,48,48	0
6	CL	D	617	1/1	0.83	0.24	62,62,62,62	0
5	GOL	D	609	6/6	0.83	0.32	76,77,78,80	0
5	GOL	C	607	6/6	0.84	0.27	29,31,34,36	0
4	SO4	D	605	5/5	0.85	0.33	122,123,124,124	0
6	CL	D	612	1/1	0.86	0.27	48,48,48,48	0
5	GOL	A	612	6/6	0.87	0.33	34,36,37,39	0
6	CL	A	610	1/1	0.87	0.14	42,42,42,42	0
5	GOL	C	609	6/6	0.88	0.24	25,26,27,27	0
5	GOL	C	608	6/6	0.88	0.23	29,33,35,35	0
5	GOL	C	606	6/6	0.88	0.21	24,25,27,28	0
5	GOL	A	607	6/6	0.89	0.22	35,42,43,46	0
6	CL	B	612	1/1	0.89	0.20	54,54,54,54	0
4	SO4	B	606	5/5	0.89	0.24	65,67,68,68	0
4	SO4	A	605	5/5	0.89	0.33	105,106,106,106	0
6	CL	D	613	1/1	0.89	0.14	38,38,38,38	0
3	BG6	D	602	16/16	0.90	0.26	64,80,87,90	0
3	BG6	C	602	16/16	0.90	0.26	73,81,86,87	0
6	CL	B	613	1/1	0.90	0.13	57,57,57,57	0
4	SO4	A	604	5/5	0.90	0.15	75,78,79,81	0
6	CL	B	610	1/1	0.90	0.17	46,46,46,46	0
5	GOL	D	608	6/6	0.91	0.31	14,28,30,32	0
5	GOL	D	607	6/6	0.91	0.18	22,29,30,31	0
3	BG6	A	601	16/16	0.91	0.22	68,73,76,79	0

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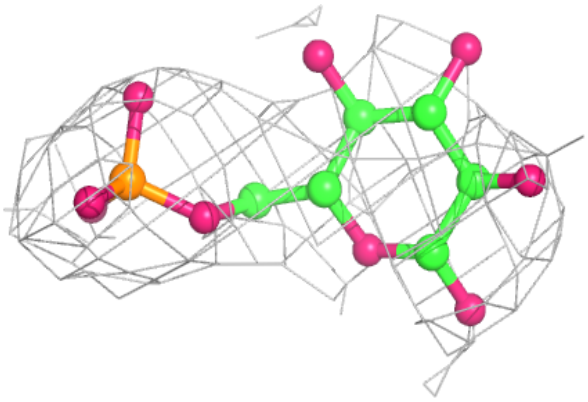
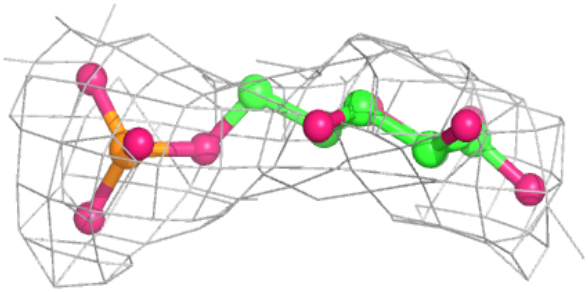
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	D	601	1/1	0.91	0.15	41,41,41,41	0
3	BG6	B	602	16/16	0.92	0.20	70,72,75,76	0
6	CL	C	611	1/1	0.92	0.11	37,37,37,37	0
6	CL	D	615	1/1	0.92	0.08	48,48,48,48	0
6	CL	D	611	1/1	0.92	0.18	56,56,56,56	0
4	SO4	B	605	5/5	0.93	0.19	59,62,63,64	0
5	GOL	A	608	6/6	0.93	0.22	31,38,39,42	0
6	CL	C	613	1/1	0.93	0.10	32,32,32,32	0
5	GOL	C	601	6/6	0.93	0.27	32,33,33,33	0
4	SO4	B	607	5/5	0.93	0.18	71,71,73,74	0
6	CL	C	610	1/1	0.93	0.13	32,32,32,32	0
5	GOL	B	608	6/6	0.94	0.18	29,34,35,36	0
6	CL	A	609	1/1	0.94	0.13	38,38,38,38	0
4	SO4	B	604	5/5	0.95	0.17	34,35,40,40	0
5	GOL	C	616	6/6	0.96	0.17	26,28,30,32	0
6	CL	D	616	1/1	0.97	0.13	44,44,44,44	0
6	CL	B	611	1/1	0.97	0.18	42,42,42,42	0
4	SO4	A	606	5/5	0.97	0.11	61,61,61,62	0
4	SO4	C	603	5/5	0.98	0.09	36,38,38,40	0
6	CL	B	609	1/1	0.98	0.07	19,19,19,19	0
6	CL	C	615	1/1	0.98	0.09	52,52,52,52	0
4	SO4	D	603	5/5	0.98	0.12	40,41,42,45	0
4	SO4	B	603	5/5	0.99	0.11	26,29,30,32	0
4	SO4	C	604	5/5	0.99	0.14	44,44,45,46	0
4	SO4	A	603	5/5	0.99	0.11	50,50,51,53	0
4	SO4	A	602	5/5	0.99	0.09	37,38,38,41	0

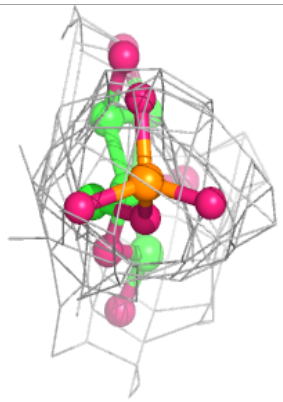
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BG6 D 602:

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

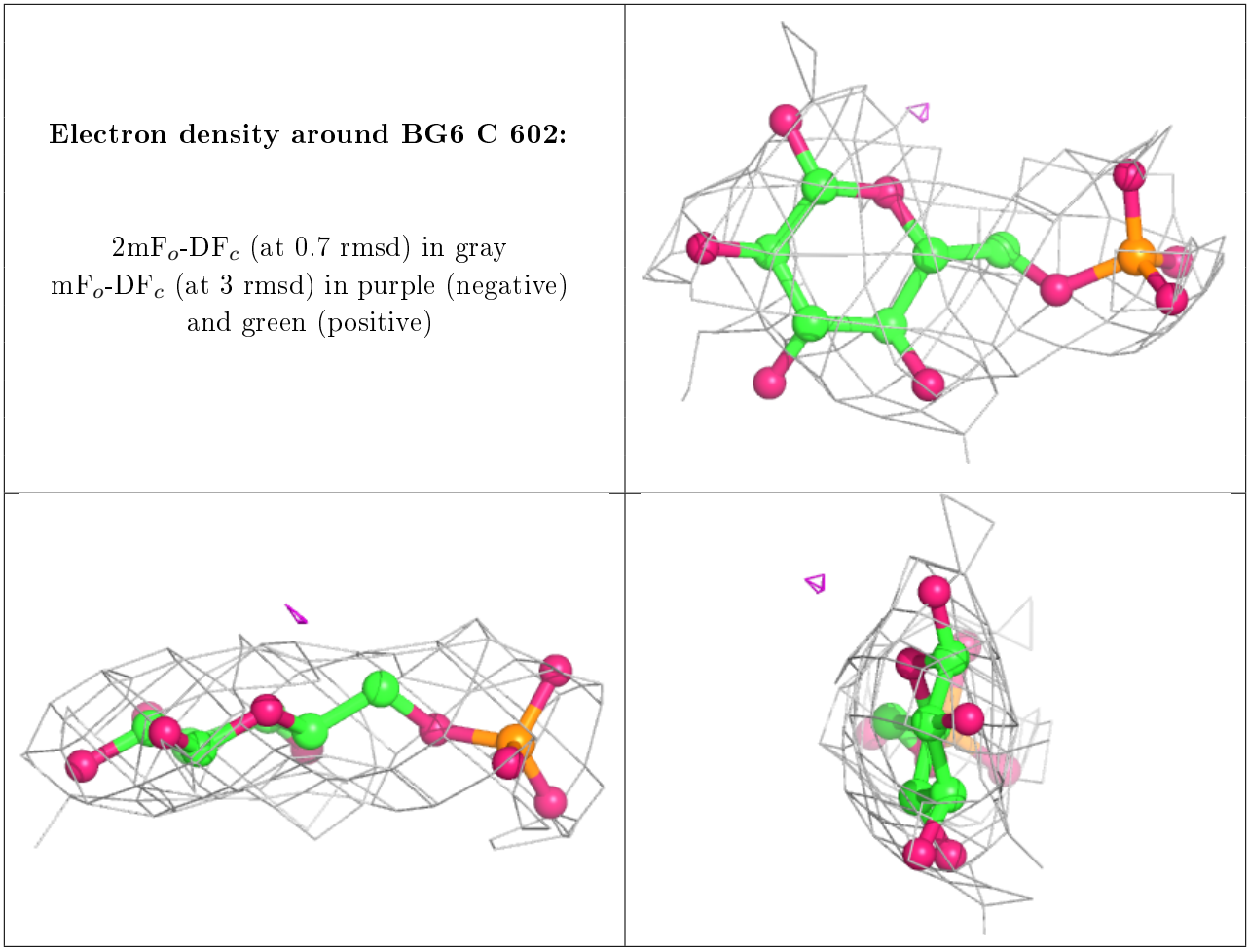






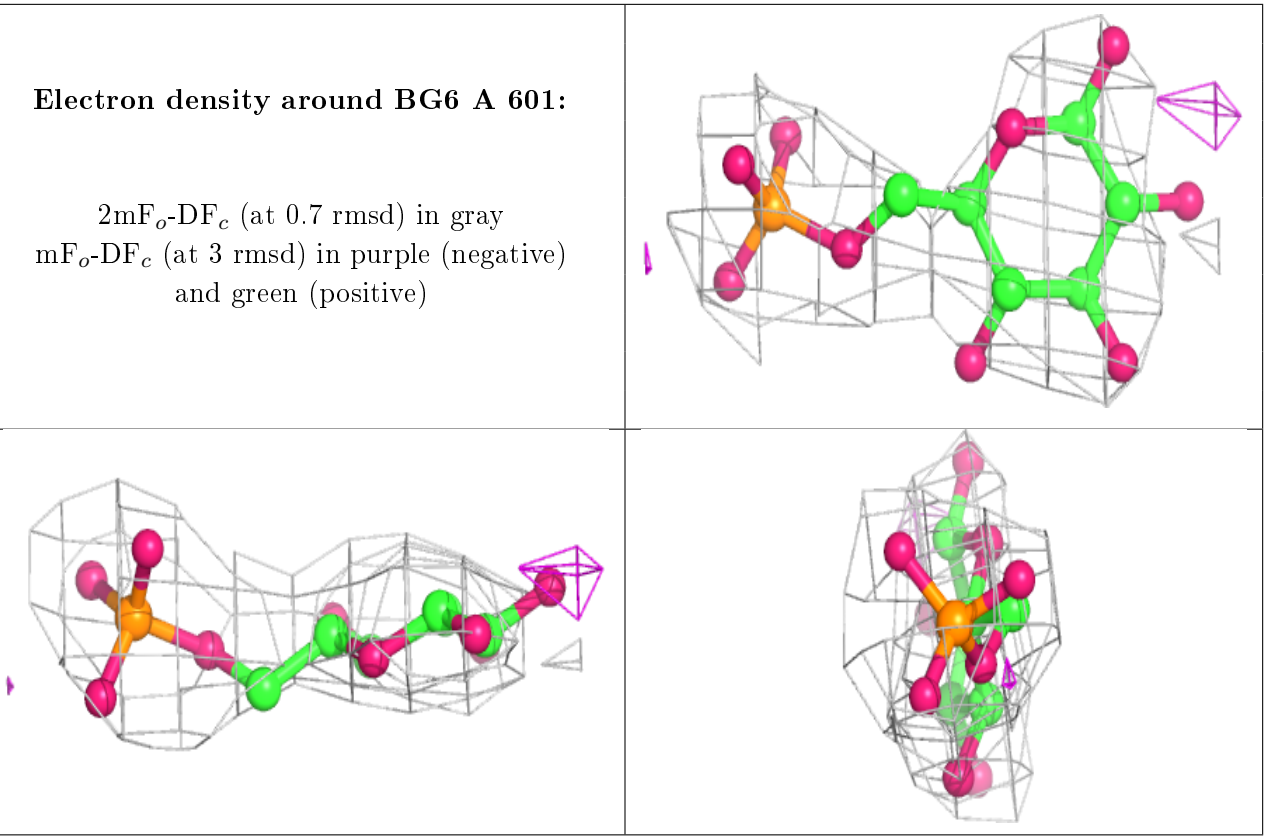
Electron density around BG6 C 602:

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



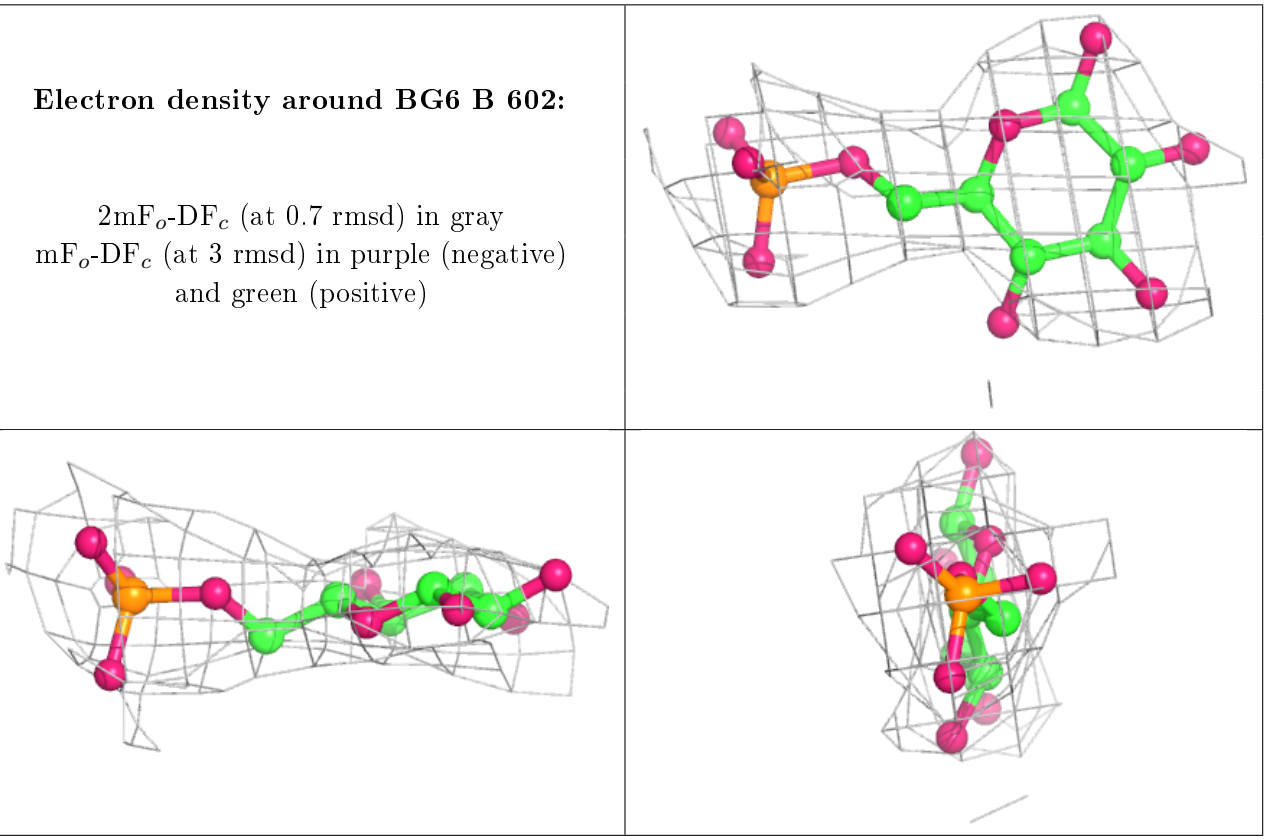
Electron density around BG6 A 601:

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



Electron density around BG6 B 602:

$2mF_o$-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.