



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:22 PM UTC

PDB ID : 6D24 / pdb_00006d24
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 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

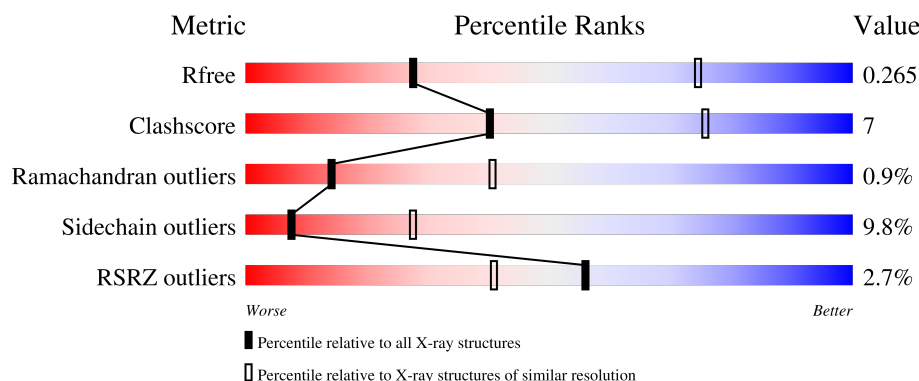
1 Overall quality at a glance

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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	541	 3% 66% 23% 7%
1	B	541	 3% 68% 22% 7%
2	C	541	 2% 68% 20% 9%
2	D	541	 2% 67% 21% 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 criteria:

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:

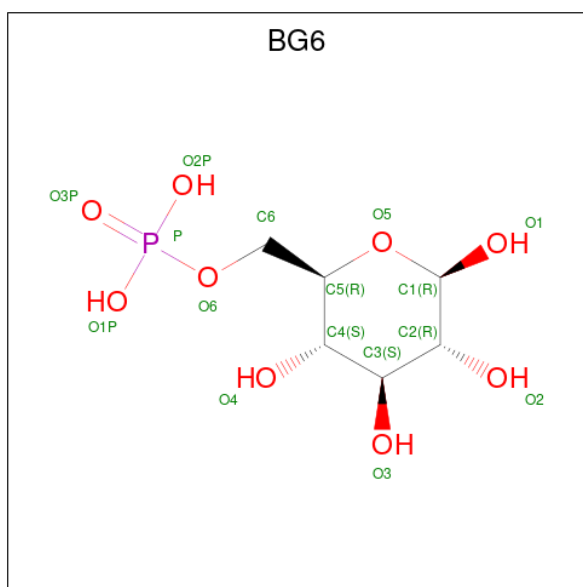
Chain	Residue	Modelled	Actual	Comment	Reference
C	15	MET	-	expression tag	UNP Q1WBU6
C	16	GLY	-	expression tag	UNP Q1WBU6
C	17	SER	-	expression tag	UNP Q1WBU6
C	18	SER	-	expression tag	UNP Q1WBU6
C	19	HIS	-	expression tag	UNP Q1WBU6
C	20	HIS	-	expression tag	UNP Q1WBU6
C	21	HIS	-	expression tag	UNP Q1WBU6

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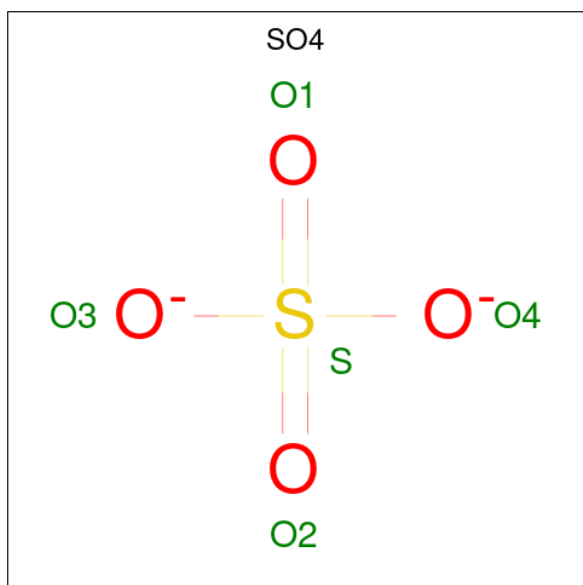
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	HIS	-	expression tag	UNP Q1WBU6
C	23	HIS	-	expression tag	UNP Q1WBU6
C	24	HIS	-	expression tag	UNP Q1WBU6
C	25	SER	-	expression tag	UNP Q1WBU6
C	26	SER	-	expression tag	UNP Q1WBU6
C	27	GLY	-	expression tag	UNP Q1WBU6
C	28	LEU	-	expression tag	UNP Q1WBU6
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 (CCD ID: BG6) (formula: C₆H₁₃O₉P).



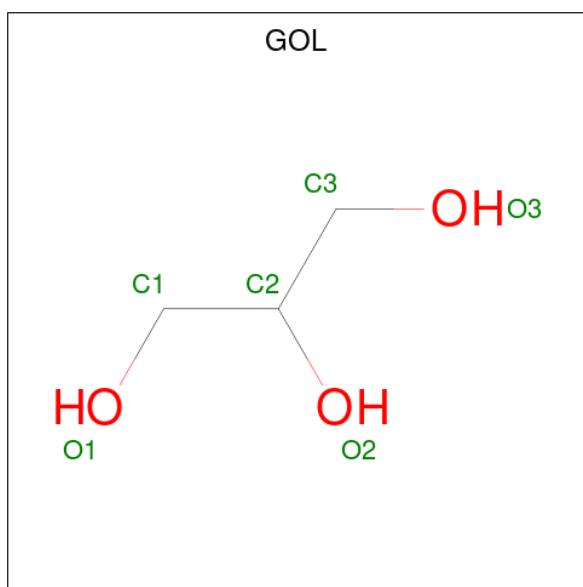
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is SULFATE ION (CCD ID: 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	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
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

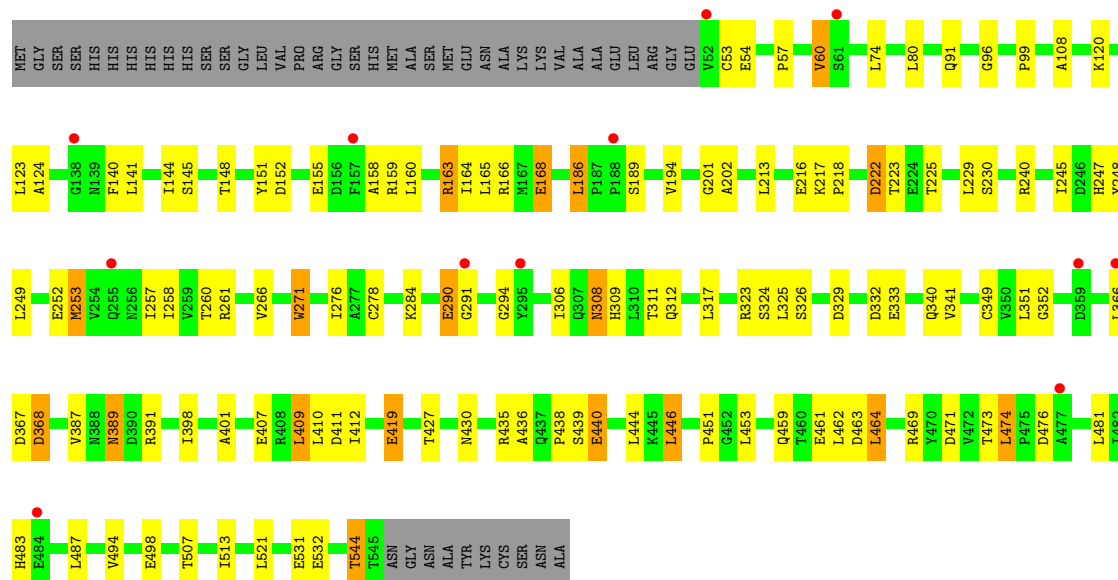
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Cl 3	0	0
6	B	6	Total 6	Cl 6	0	0
6	C	6	Total 6	Cl 6	0	0
6	D	8	Total 8	Cl 8	0	0

- Molecule 7 is water.

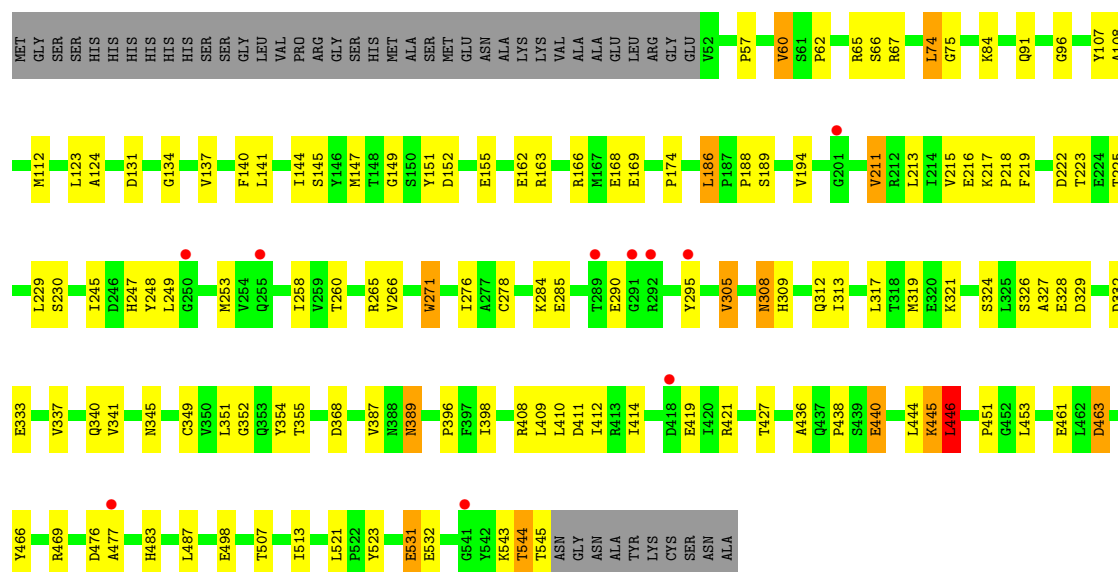
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total 8	O 8	0	0
7	B	9	Total 9	O 9	0	0
7	C	17	Total 17	O 17	0	0
7	D	13	Total 13	O 13	0	0



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



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



4 Data and refinement statistics

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 34.16 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.16-3.35) 99.3 (34.16-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.32Å)	Xtrriage
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	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: CSO, BG6, CL, SO4, GOL

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	0.88	1/4002 (0.0%)	1.42	44/5432 (0.8%)
1	B	0.90	2/4041 (0.0%)	1.42	43/5477 (0.8%)
2	C	0.87	0/3983	1.41	26/5397 (0.5%)
2	D	0.88	0/3984	1.41	27/5398 (0.5%)
All	All	0.88	3/16010 (0.0%)	1.41	140/21704 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	543	LYS	CA-C	7.88	1.57	1.53
1	A	56	ILE	CA-C	5.31	1.58	1.52
1	B	545	THR	CA-C	5.07	1.59	1.52

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	463	ASP	CA-CB-CG	8.76	121.36	112.60
2	D	411	ASP	CA-CB-CG	8.68	121.28	112.60
2	C	411	ASP	CA-CB-CG	8.53	121.13	112.60
1	A	411	ASP	CA-CB-CG	8.14	120.74	112.60
1	B	411	ASP	CA-CB-CG	8.11	120.71	112.60
2	D	419	GLU	CA-C-N	7.62	130.75	120.77
2	D	419	GLU	C-N-CA	7.62	130.75	120.77
1	A	235	PRO	CA-C-N	7.44	130.25	120.28
1	A	235	PRO	C-N-CA	7.44	130.25	120.28
1	A	419	GLU	CA-C-N	7.43	130.50	120.77
1	A	419	GLU	C-N-CA	7.43	130.50	120.77
1	B	419	GLU	CA-C-N	7.42	130.50	120.77
1	B	419	GLU	C-N-CA	7.42	130.50	120.77
1	B	476	ASP	CA-CB-CG	7.28	119.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ASP	CA-CB-CG	7.28	119.88	112.60
2	C	419	GLU	CA-C-N	7.10	129.76	120.60
2	C	419	GLU	C-N-CA	7.10	129.76	120.60
2	C	54	GLU	CA-C-N	6.88	130.60	120.90
2	C	54	GLU	C-N-CA	6.88	130.60	120.90
2	C	163	ARG	CA-C-N	6.88	129.23	120.56
2	C	163	ARG	C-N-CA	6.88	129.23	120.56
1	A	152	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	543	LYS	CA-C-N	6.62	134.19	121.54
1	B	543	LYS	C-N-CA	6.62	134.19	121.54
2	C	476	ASP	CA-CB-CG	6.62	119.22	112.60
2	C	463	ASP	CA-C-N	6.57	130.53	121.33
2	C	463	ASP	C-N-CA	6.57	130.53	121.33
1	B	112	MET	CA-C-N	6.54	130.69	120.89
1	B	112	MET	C-N-CA	6.54	130.69	120.89
1	B	152	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	547	GLY	CA-C-N	6.43	128.79	120.44
1	B	547	GLY	C-N-CA	6.43	128.79	120.44
1	B	113	GLU	CB-CG-CD	6.41	123.49	112.60
2	D	476	ASP	CA-CB-CG	6.39	119.00	112.60
1	B	368	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	543	LYS	N-CA-C	6.28	114.77	108.75
2	D	368	ASP	CA-CB-CG	6.26	118.86	112.60
2	C	222	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	332	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	544	THR	CA-C-N	6.06	133.12	121.54
1	B	544	THR	C-N-CA	6.06	133.12	121.54
2	D	152	ASP	CA-CB-CG	6.05	118.65	112.60
2	D	75	GLY	CA-C-N	6.04	129.49	120.31
2	D	75	GLY	C-N-CA	6.04	129.49	120.31
2	D	163	ARG	CA-C-N	6.01	128.70	120.46
2	D	163	ARG	C-N-CA	6.01	128.70	120.46
2	C	152	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	543	LYS	CA-C-N	5.94	132.89	121.54
1	A	543	LYS	C-N-CA	5.94	132.89	121.54
1	A	368	ASP	CA-CB-CG	5.94	118.54	112.60
2	D	211	VAL	N-CA-CB	5.93	119.59	111.41
1	A	548	ASN	CA-C-N	5.93	132.11	122.39
1	A	548	ASN	C-N-CA	5.93	132.11	122.39
1	A	131	ASP	N-CA-C	-5.91	105.73	113.17
2	C	368	ASP	CA-CB-CG	5.90	118.50	112.60
2	D	327	ALA	CA-C-N	5.84	128.69	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	327	ALA	C-N-CA	5.84	128.69	120.28
2	D	543	LYS	CA-C-N	5.83	132.68	121.54
2	D	543	LYS	C-N-CA	5.83	132.68	121.54
1	A	548	ASN	N-CA-C	5.81	117.88	108.41
1	B	188	PRO	CA-C-N	5.81	128.65	120.28
1	B	188	PRO	C-N-CA	5.81	128.65	120.28
1	A	289	THR	CA-C-N	5.70	132.44	121.54
1	A	289	THR	C-N-CA	5.70	132.44	121.54
2	C	332	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	389	ASN	CA-CB-CG	5.67	118.27	112.60
2	D	188	PRO	CA-C-N	5.65	128.41	120.28
2	D	188	PRO	C-N-CA	5.65	128.41	120.28
2	D	389	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	550	TYR	CA-C-N	5.58	128.22	120.63
1	A	550	TYR	C-N-CA	5.58	128.22	120.63
1	B	471	ASP	CA-C-N	5.58	130.29	123.10
1	B	471	ASP	C-N-CA	5.58	130.29	123.10
2	D	332	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	309	HIS	N-CA-C	5.53	116.98	111.07
2	D	463	ASP	CA-C-N	5.51	132.06	121.54
2	D	463	ASP	C-N-CA	5.51	132.06	121.54
1	A	265	ARG	CA-C-N	5.48	127.46	120.56
1	A	265	ARG	C-N-CA	5.48	127.46	120.56
1	A	313	ILE	CA-C-N	5.47	127.61	120.28
1	A	313	ILE	C-N-CA	5.47	127.61	120.28
2	C	311	THR	N-CA-C	-5.46	105.49	111.82
1	B	446	LEU	N-CA-CB	-5.45	102.22	111.69
1	A	231	ASN	CA-C-N	5.44	128.12	120.28
1	A	231	ASN	C-N-CA	5.44	128.12	120.28
2	D	265	ARG	CA-C-N	5.44	127.41	120.56
2	D	265	ARG	C-N-CA	5.44	127.41	120.56
1	B	530	PRO	CA-C-N	5.42	127.81	120.38
1	B	530	PRO	C-N-CA	5.42	127.81	120.38
1	B	239	GLU	CA-C-N	5.39	127.77	120.38
1	B	239	GLU	C-N-CA	5.39	127.77	120.38
1	A	382	VAL	N-CA-CB	5.39	119.15	111.82
1	A	474	LEU	N-CA-C	5.39	115.80	109.60
2	C	474	LEU	N-CA-C	5.36	115.76	109.60
1	B	359	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	474	LEU	N-CA-C	5.33	115.73	109.60
2	D	328	GLU	CB-CG-CD	5.31	121.62	112.60
1	B	306	ILE	CA-C-N	5.30	127.81	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ILE	C-N-CA	5.30	127.81	120.29
2	C	294	GLY	CA-C-N	5.29	127.81	120.29
2	C	294	GLY	C-N-CA	5.29	127.81	120.29
1	A	456	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	309	HIS	N-CA-C	5.25	116.69	111.07
1	B	550	TYR	CA-C-N	5.25	127.77	120.63
1	B	550	TYR	C-N-CA	5.25	127.77	120.63
1	A	389	ASN	CA-CB-CG	5.24	117.83	112.60
2	D	446	LEU	N-CA-CB	-5.22	102.95	111.66
1	A	188	PRO	CA-C-N	5.20	128.92	120.60
1	A	188	PRO	C-N-CA	5.20	128.92	120.60
1	B	332	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	382	VAL	N-CA-CB	5.18	119.08	111.52
2	C	409	LEU	N-CA-C	5.17	116.80	108.32
1	A	239	GLU	CA-C-N	5.17	127.47	120.38
1	A	239	GLU	C-N-CA	5.17	127.47	120.38
1	B	497	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	531	GLU	CA-C-N	5.16	127.45	120.38
1	A	531	GLU	C-N-CA	5.16	127.45	120.38
1	A	75	GLY	CA-C-N	5.16	127.71	120.28
1	A	75	GLY	C-N-CA	5.16	127.71	120.28
1	B	551	LYS	CA-C-N	5.14	128.52	120.75
1	B	551	LYS	C-N-CA	5.14	128.52	120.75
2	C	158	ALA	N-CA-C	-5.13	105.76	111.36
2	C	473	THR	CA-C-N	5.11	127.92	120.51
2	C	473	THR	C-N-CA	5.11	127.92	120.51
1	B	265	ARG	CA-C-N	5.10	127.18	120.60
1	B	265	ARG	C-N-CA	5.10	127.18	120.60
2	D	531	GLU	CA-C-N	5.09	127.36	120.38
2	D	531	GLU	C-N-CA	5.09	127.36	120.38
1	A	175	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	75	GLY	CA-C-N	5.09	128.74	120.60
1	B	75	GLY	C-N-CA	5.09	128.74	120.60
1	A	551	LYS	CA-C-N	5.08	128.43	120.75
1	A	551	LYS	C-N-CA	5.08	128.43	120.75
1	A	82	LYS	CB-CA-C	-5.08	102.90	110.88
1	B	548	ASN	N-CA-C	5.08	116.51	111.07
1	A	473	THR	CA-C-N	5.07	127.86	120.51
1	A	473	THR	C-N-CA	5.07	127.86	120.51
2	C	389	ASN	CA-CB-CG	5.02	117.62	112.60
2	C	531	GLU	CA-C-N	5.02	127.26	120.38
2	C	531	GLU	C-N-CA	5.02	127.26	120.38

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	61	0
1	B	3960	0	3905	46	0
2	C	3910	0	3872	54	0
2	D	3911	0	3872	62	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
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	207	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 7.

All (207) 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:253:MET:HE3	1:A:440:GLU:HB3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:LYS:HE3	5:D:610:GOL:H12	1.93	0.50
2:D:134:GLY:O	2:D:137:VAL:HG12	2.11	0.50
1:B:341:VAL:HG22	1:B:387:VAL:HG22	1.92	0.50
2:C:253:MET:HE3	2:C:440:GLU:HB3	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
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:B:415:GLN:HG3	1:B:431:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:341:VAL:HG22	2:C:387:VAL:HG22	1.98	0.46
1:A:166:ARG:HH21	1:A:169:GLU:CD	2.24	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
1:A:56:ILE:HG13	1:A:56:ILE:O	2.16	0.45
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:A:267:PHE:CE2	2:D:446:LEU:HD11	2.51	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: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
1:B:366:LEU:C	1:B:368:ASP:H	2.25	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
1:A:366:LEU:C	1:A:368:ASP:H	2.26	0.44
2:C:160:LEU:HG	2:C:164:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:LEU:C	2:C:368:ASP:H	2.26	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:A:319:MET:HE3	1:A:333:GLU:HB2	1.99	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
1:B:147:MET:HE1	1:B:159:ARG:C	2.44	0.43
2:C:308:ASN:ND2	2:C:309:HIS:H	2.17	0.43
2:D:532:GLU:H	2:D:532:GLU:CD	2.27	0.43
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:C:532:GLU:CD	2:C:532:GLU:H	2.26	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:72:VAL:HG12	1:B:74:LEU:HD22	2.02	0.42
1:B:350:VAL:HB	1:B:382:VAL:HG22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:532:GLU:H	1:A:532:GLU:CD	2.27	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
1:A:500:ASP:CG	1:A:504:ARG:HE	2.29	0.41
2:C:60:VAL:HG11	2:C:99:PRO:HA	2.02	0.41
2:D:147:MET:HE3	2:D:147:MET:HB2	1.90	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:532:GLU:CD	1:B:532:GLU:H	2.28	0.41
1:A:422:PRO:HD3	2:D:321:LYS:HD3	2.02	0.41
1:B:72:VAL:HG11	1:B:160:LEU:HD11	2.03	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
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
2:D:66:SER:O	2:D:174:PRO:HD2	2.21	0.41
1:A:216:GLU:HA	1:A:245:ILE:HG22	2.03	0.41
2:C:306:ILE:HD11	2:C:401:ALA:HB3	2.03	0.41
1:B:549:ALA:H	1:B:552:CYS:HB2	1.86	0.41
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:HD23	2:C:325:LEU:HA	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:278:CYS:SG	1:B:398:ILE:HD12	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	12	38
1	B	502/541 (93%)	456 (91%)	40 (8%)	6 (1%)	10	33
2	C	492/541 (91%)	454 (92%)	33 (7%)	5 (1%)	12	38
2	D	492/541 (91%)	459 (93%)	31 (6%)	2 (0%)	30	58
All	All	1988/2164 (92%)	1833 (92%)	137 (7%)	18 (1%)	14	41

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLU
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

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Mol	Chain	Res	Type
2	C	438	PRO
2	D	438	PRO
1	B	367	ASP
1	A	177	GLY

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	414/462 (90%)	372 (90%)	42 (10%)	7	26
1	B	421/462 (91%)	382 (91%)	39 (9%)	8	30
2	C	417/461 (90%)	379 (91%)	38 (9%)	9	30
2	D	419/461 (91%)	375 (90%)	44 (10%)	6	24
All	All	1671/1846 (90%)	1508 (90%)	163 (10%)	7	27

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	56	ILE
1	A	67	ARG
1	A	74	LEU
1	A	91	GLN
1	A	105	LEU
1	A	123	LEU
1	A	131	ASP
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

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Mol	Chain	Res	Type
1	A	213	LEU
1	A	225	THR
1	A	229	LEU
1	A	230	SER
1	A	233	LEU
1	A	240	ARG
1	A	253	MET
1	A	258	ILE
1	A	260	THR
1	A	271	TRP
1	A	285	GLU
1	A	290	GLU
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	362	THR
1	A	366	LEU
1	A	427	THR
1	A	440	GLU
1	A	453	LEU
1	A	454	LEU
1	A	463	ASP
1	B	53	CYS
1	B	67	ARG
1	B	91	GLN
1	B	101	ASP
1	B	145	SER
1	B	155	GLU
1	B	160	LEU
1	B	186	LEU
1	B	189	SER
1	B	207	GLU
1	B	213	LEU
1	B	222	ASP
1	B	225	THR
1	B	229	LEU
1	B	230	SER
1	B	233	LEU
1	B	240	ARG

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Mol	Chain	Res	Type
1	B	253	MET
1	B	258	ILE
1	B	260	THR
1	B	271	TRP
1	B	285	GLU
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	427	THR
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	534	GLN
2	C	53	CYS
2	C	60	VAL
2	C	74	LEU
2	C	91	GLN
2	C	123	LEU
2	C	145	SER
2	C	155	GLU
2	C	159	ARG
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
2	C	230	SER
2	C	240	ARG
2	C	253	MET
2	C	258	ILE

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Mol	Chain	Res	Type
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	349	CYS
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	494	VAL
2	C	498	GLU
2	C	544	THR
2	D	60	VAL
2	D	67	ARG
2	D	74	LEU
2	D	91	GLN
2	D	112	MET
2	D	123	LEU
2	D	131	ASP
2	D	145	SER
2	D	155	GLU
2	D	168	GLU
2	D	169	GLU
2	D	186	LEU
2	D	189	SER
2	D	211	VAL
2	D	213	LEU
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
2	D	285	GLU

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Mol	Chain	Res	Type
2	D	290	GLU
2	D	295	TYR
2	D	305	VAL
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	445	LYS
2	D	446	LEU
2	D	453	LEU
2	D	461	GLU
2	D	463	ASP
2	D	498	GLU
2	D	531	GLU
2	D	544	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	136	HIS
1	A	228	GLN
1	A	232	GLN
1	A	280	GLN
1	A	308	ASN
1	A	340	GLN
1	A	345	ASN
1	A	388	ASN
1	B	307	GLN
1	B	388	ASN
2	C	91	GLN
2	C	95	ASN
2	C	247	HIS
2	C	272	ASN
2	C	307	GLN
2	C	340	GLN
2	C	388	ASN

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Mol	Chain	Res	Type
2	D	91	GLN
2	D	232	GLN
2	D	238	ASN
2	D	272	ASN
2	D	307	GLN
2	D	308	ASN
2	D	312	GLN
2	D	340	GLN
2	D	483	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	528	2	3,6,7	0.61	0	1,6,8	0.68	0
2	CSO	C	528	2	3,6,7	0.81	0	1,6,8	0.95	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
2	CSO	D	528	2	-	0/1/5/7	-
2	CSO	C	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 oligosaccharides 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	$\# Z > 2$
4	SO4	B	604	-	4,4,4	0.24	0	6,6,6	0.45	0
3	BG6	D	602	-	16,16,16	0.40	0	23,24,24	0.59	0
4	SO4	B	603	-	4,4,4	0.31	0	6,6,6	0.28	0
3	BG6	B	602	-	16,16,16	0.44	0	23,24,24	0.64	0
5	GOL	B	608	-	5,5,5	0.15	0	5,5,5	0.25	0
4	SO4	D	603	-	4,4,4	0.34	0	6,6,6	0.31	0
5	GOL	A	608	-	5,5,5	0.12	0	5,5,5	0.22	0
4	SO4	C	605	-	4,4,4	0.28	0	6,6,6	0.15	0
5	GOL	D	609	-	5,5,5	0.10	0	5,5,5	0.24	0
4	SO4	A	604	-	4,4,4	0.20	0	6,6,6	0.23	0
4	SO4	B	607	-	4,4,4	0.25	0	6,6,6	0.22	0
5	GOL	C	608	-	5,5,5	0.16	0	5,5,5	0.72	0
5	GOL	D	607	-	5,5,5	0.19	0	5,5,5	0.25	0
5	GOL	C	609	-	5,5,5	0.14	0	5,5,5	0.27	0
4	SO4	C	603	-	4,4,4	0.19	0	6,6,6	0.19	0
3	BG6	C	602	-	16,16,16	0.54	0	23,24,24	0.59	0
5	GOL	D	608	-	5,5,5	0.25	0	5,5,5	0.28	0
5	GOL	C	601	-	5,5,5	0.13	0	5,5,5	0.31	0
5	GOL	C	616	-	5,5,5	0.12	0	5,5,5	0.19	0
4	SO4	A	606	-	4,4,4	0.28	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	606	-	5,5,5	0.19	0	5,5,5	0.42	0
5	GOL	A	612	-	5,5,5	0.19	0	5,5,5	0.42	0
5	GOL	C	607	-	5,5,5	0.21	0	5,5,5	0.51	0
4	SO4	D	605	-	4,4,4	0.31	0	6,6,6	0.14	0
3	BG6	A	601	-	16,16,16	0.36	0	23,24,24	0.44	0
4	SO4	A	602	-	4,4,4	0.31	0	6,6,6	0.21	0
4	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.32	0
4	SO4	C	604	-	4,4,4	0.29	0	6,6,6	0.23	0
4	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.28	0
4	SO4	D	606	-	4,4,4	0.37	0	6,6,6	0.28	0
4	SO4	A	605	-	4,4,4	0.30	0	6,6,6	0.17	0
4	SO4	B	606	-	4,4,4	0.37	0	6,6,6	0.19	0
5	GOL	A	607	-	5,5,5	0.16	0	5,5,5	0.54	0
4	SO4	D	604	-	4,4,4	0.25	0	6,6,6	0.29	0
5	GOL	D	610	-	5,5,5	0.20	0	5,5,5	0.36	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
5	GOL	D	609	-	-	0/4/4/4	-
5	GOL	C	616	-	-	2/4/4/4	-
5	GOL	C	606	-	-	0/4/4/4	-
3	BG6	D	602	-	-	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	C	607	-	-	0/4/4/4	-
5	GOL	C	608	-	-	0/4/4/4	-
5	GOL	D	607	-	-	0/4/4/4	-
3	BG6	B	602	-	-	2/6/26/26	0/1/1/1
5	GOL	A	607	-	-	0/4/4/4	-
5	GOL	B	608	-	-	0/4/4/4	-
5	GOL	C	609	-	-	2/4/4/4	-
5	GOL	A	608	-	-	0/4/4/4	-
3	BG6	C	602	-	-	3/6/26/26	0/1/1/1
3	BG6	A	601	-	-	2/6/26/26	0/1/1/1
5	GOL	C	601	-	-	0/4/4/4	-
5	GOL	D	610	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	BG6	O5-C5-C6-O6
3	A	601	BG6	C4-C5-C6-O6
3	B	602	BG6	C4-C5-C6-O6
3	C	602	BG6	O5-C5-C6-O6
3	C	602	BG6	C4-C5-C6-O6
3	D	602	BG6	O5-C5-C6-O6
3	D	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	C	616	GOL	O1-C1-C2-C3
5	D	610	GOL	O1-C1-C2-C3
5	C	616	GOL	O1-C1-C2-O2
3	B	602	BG6	O5-C5-C6-O6
5	C	609	GOL	O1-C1-C2-O2
3	C	602	BG6	C6-O6-P-O3P

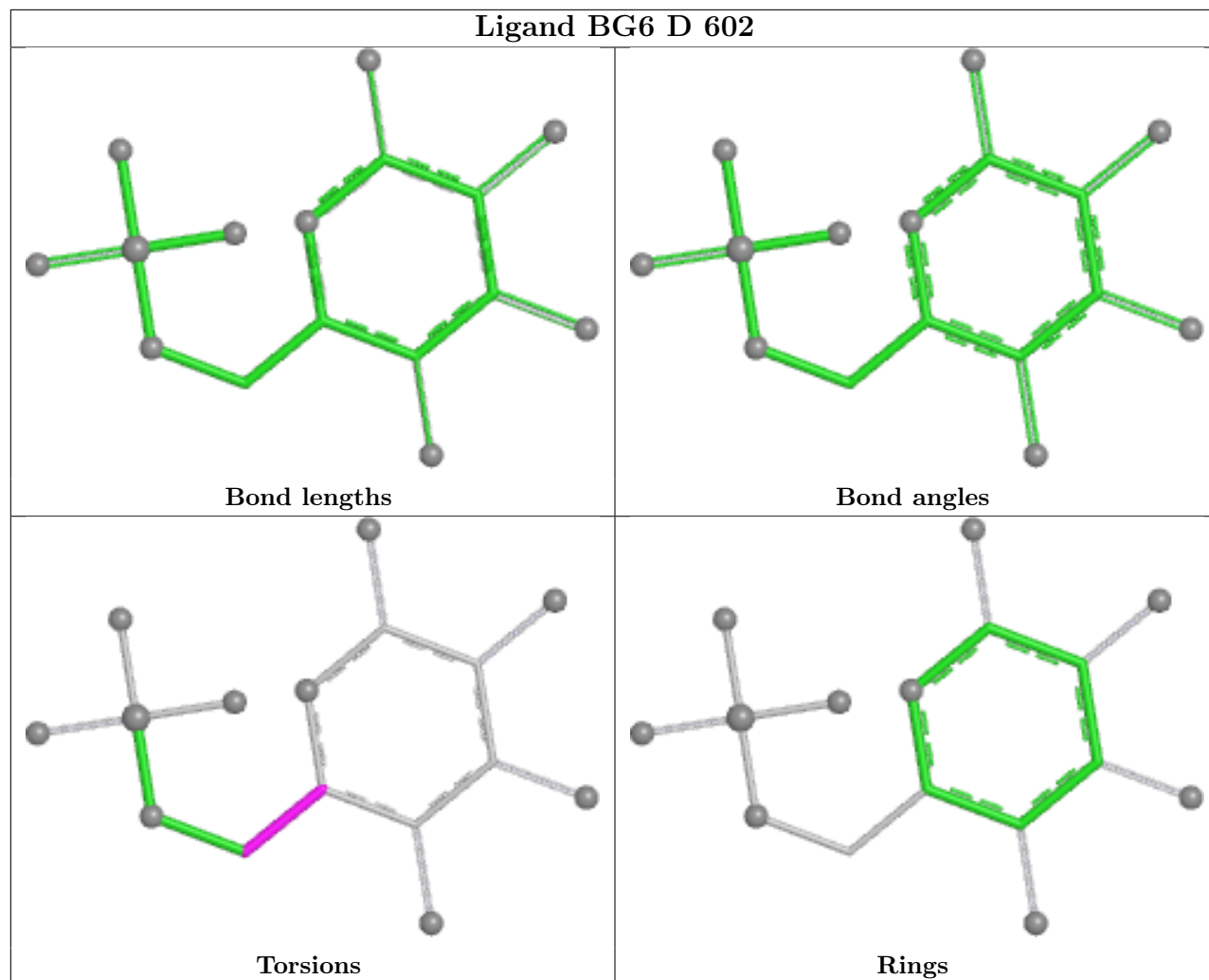
There are no ring outliers.

4 monomers are involved in 7 short contacts:

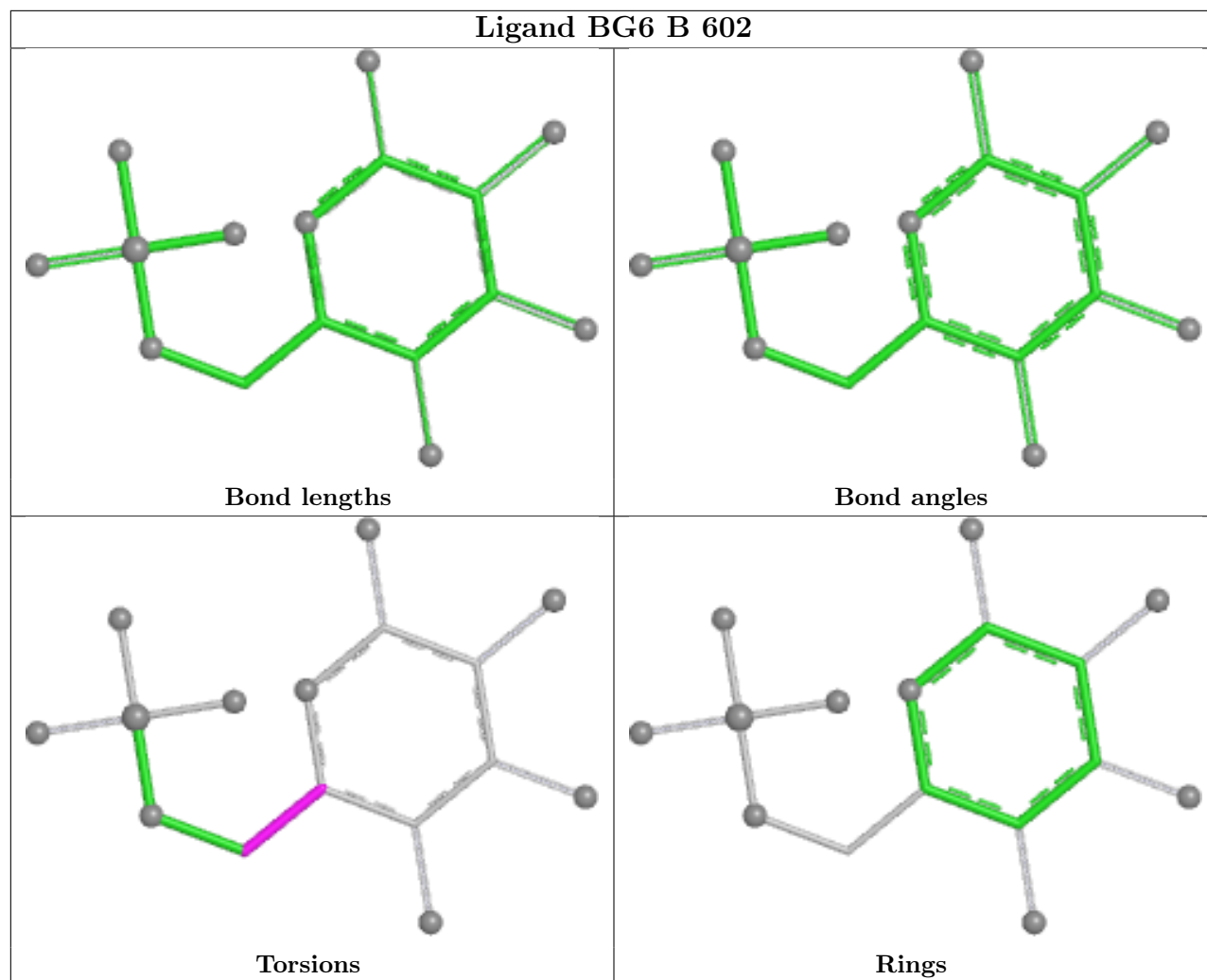
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	BG6	1	0
5	C	607	GOL	1	0
5	A	607	GOL	4	0
5	D	610	GOL	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

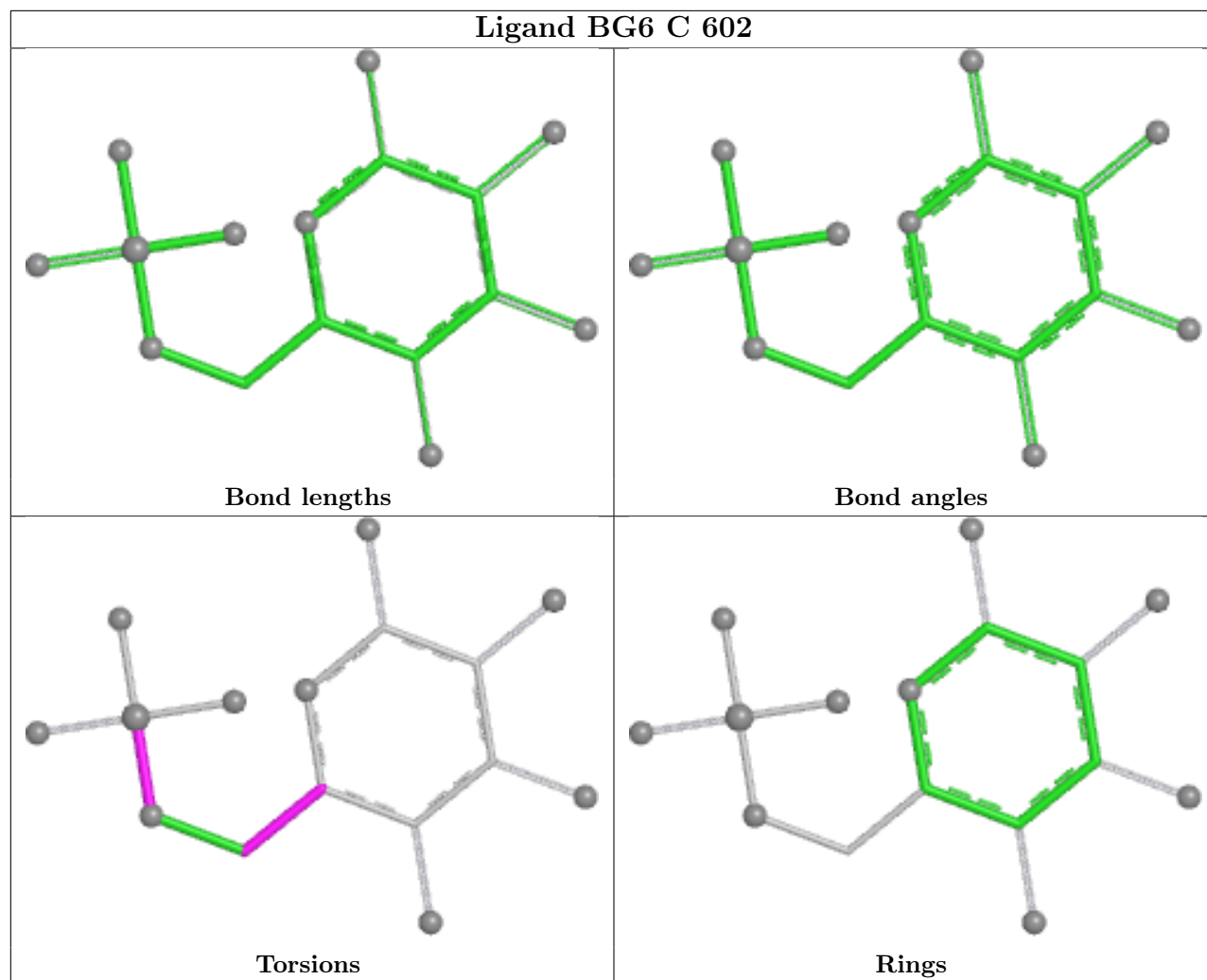
equivalents in the CSD to analyse the geometry.

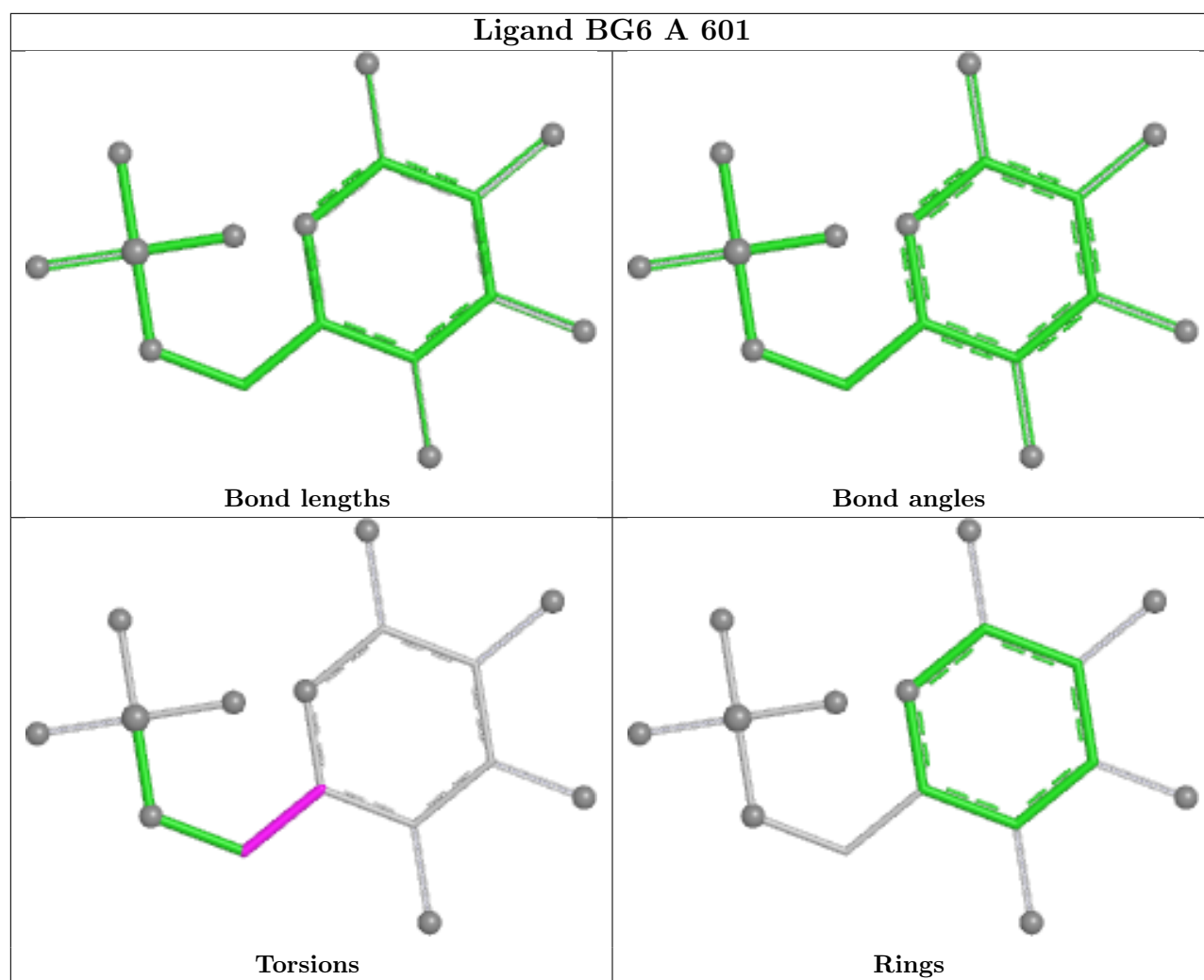


Ligand BG6 B 602



Ligand BG6 C 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	502/541 (92%)	0.41	17 (3%) 48 34	9, 35, 73, 98	2 (0%)
1	B	502/541 (92%)	0.31	15 (2%) 52 38	10, 33, 71, 93	2 (0%)
2	C	493/541 (91%)	0.42	12 (2%) 59 44	7, 33, 71, 89	1 (0%)
2	D	493/541 (91%)	0.34	10 (2%) 65 48	6, 33, 69, 83	1 (0%)
All	All	1990/2164 (91%)	0.37	54 (2%) 56 41	6, 33, 71, 98	6 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455[A]	ASN	6.1
1	A	295[A]	TYR	4.5
2	C	477	ALA	4.4
1	B	467[A]	GLU	4.1
1	B	546	ASN	4.0
2	D	201	GLY	3.9
1	A	418[A]	ASP	3.5
2	C	138	GLY	3.3
2	C	295	TYR	3.2
1	B	550	TYR	3.1
1	A	258	ILE	3.0
2	D	250	GLY	2.9
2	C	484	GLU	2.9
1	A	549	ALA	2.8
2	D	418[A]	ASP	2.8
2	D	477	ALA	2.7
1	A	550	TYR	2.7
1	B	52	VAL	2.7
2	D	289	THR	2.7
1	A	167	MET	2.6
1	B	121	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	374	GLY	2.6
1	A	52	VAL	2.5
1	A	546	ASN	2.5
1	B	128	THR	2.5
1	B	549	ALA	2.4
2	D	541	GLY	2.4
2	C	157	PHE	2.4
1	B	59	ALA	2.4
2	C	366	LEU	2.3
1	B	54	GLU	2.3
1	A	55	ARG	2.3
2	C	255	GLN	2.3
2	C	52	VAL	2.3
2	D	292	ARG	2.3
1	A	553	SER	2.3
1	A	202	ALA	2.2
1	B	206	PRO	2.2
2	D	291	GLY	2.2
1	B	553	SER	2.2
2	D	255	GLN	2.2
1	B	130	LEU	2.2
1	A	453	LEU	2.2
1	A	157	PHE	2.2
2	C	188	PRO	2.1
2	C	359	ASP	2.1
2	C	291	GLY	2.1
1	A	548	ASN	2.1
1	B	53	CYS	2.1
2	D	295	TYR	2.1
1	B	174	PRO	2.0
2	C	61	SER	2.0
1	A	131	ASP	2.0
1	A	369	PRO	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	CSO	D	528	7/8	0.82	0.16	47,49,51,52	0
2	CSO	C	528	7/8	0.83	0.15	38,40,42,43	0

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($\text{\AA}^2$)	Q<0.9
4	SO4	D	606	5/5	0.67	0.22	82,82,83,85	0
4	SO4	D	604	5/5	0.70	0.24	78,79,80,81	0
5	GOL	A	612	6/6	0.76	0.16	34,36,37,39	0
4	SO4	C	605	5/5	0.80	0.16	92,92,93,95	0
4	SO4	A	605	5/5	0.81	0.20	105,106,106,106	0
6	CL	D	612	1/1	0.81	0.11	48,48,48,48	0
5	GOL	D	609	6/6	0.82	0.19	76,77,78,80	0
3	BG6	C	602	16/16	0.83	0.16	73,81,86,87	0
4	SO4	B	606	5/5	0.83	0.20	65,67,68,68	0
5	GOL	D	610	6/6	0.84	0.15	36,40,42,42	0
6	CL	C	612	1/1	0.85	0.09	64,64,64,64	0
4	SO4	B	605	5/5	0.86	0.12	59,62,63,64	0
6	CL	D	617	1/1	0.86	0.09	62,62,62,62	0
3	BG6	B	602	16/16	0.87	0.14	70,72,75,76	0
5	GOL	D	608	6/6	0.88	0.13	14,28,30,32	0
5	GOL	C	607	6/6	0.88	0.15	29,31,34,36	0
6	CL	D	615	1/1	0.88	0.11	48,48,48,48	0
5	GOL	C	608	6/6	0.88	0.12	29,33,35,35	0
4	SO4	B	607	5/5	0.89	0.14	71,71,73,74	0
5	GOL	A	608	6/6	0.89	0.13	31,38,39,42	0
3	BG6	D	602	16/16	0.89	0.12	64,80,87,90	0
3	BG6	A	601	16/16	0.89	0.11	68,73,76,79	0
6	CL	C	615	1/1	0.89	0.09	52,52,52,52	0
4	SO4	D	605	5/5	0.89	0.14	122,123,124,124	0
5	GOL	C	609	6/6	0.89	0.13	25,26,27,27	0
5	GOL	D	607	6/6	0.89	0.13	22,29,30,31	0
5	GOL	B	608	6/6	0.90	0.10	29,34,35,36	0

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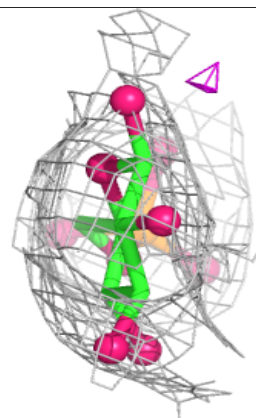
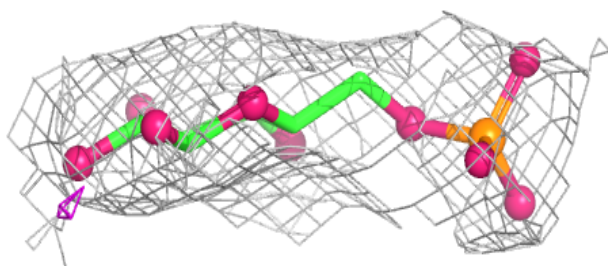
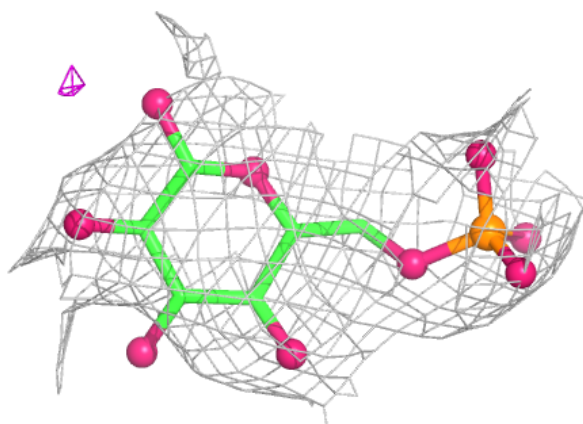
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	D	601	1/1	0.91	0.10	41,41,41,41	0
6	CL	B	601	1/1	0.91	0.13	59,59,59,59	0
5	GOL	C	606	6/6	0.91	0.13	24,25,27,28	0
4	SO4	A	604	5/5	0.91	0.10	75,78,79,81	0
5	GOL	A	607	6/6	0.92	0.16	35,42,43,46	0
4	SO4	A	606	5/5	0.92	0.11	61,61,61,62	0
5	GOL	C	601	6/6	0.92	0.15	32,33,33,33	0
6	CL	A	610	1/1	0.93	0.08	42,42,42,42	0
4	SO4	A	603	5/5	0.93	0.12	50,50,51,53	0
6	CL	B	611	1/1	0.93	0.08	42,42,42,42	0
6	CL	D	614	1/1	0.93	0.10	72,72,72,72	0
6	CL	B	612	1/1	0.93	0.10	54,54,54,54	0
4	SO4	B	604	5/5	0.93	0.13	34,35,40,40	0
6	CL	A	609	1/1	0.94	0.10	38,38,38,38	0
6	CL	C	611	1/1	0.94	0.07	37,37,37,37	0
6	CL	A	611	1/1	0.94	0.14	48,48,48,48	0
6	CL	C	614	1/1	0.95	0.06	61,61,61,61	0
6	CL	D	611	1/1	0.95	0.09	56,56,56,56	0
4	SO4	C	604	5/5	0.96	0.07	44,44,45,46	0
4	SO4	C	603	5/5	0.96	0.07	36,38,38,40	0
5	GOL	C	616	6/6	0.96	0.09	26,28,30,32	0
6	CL	D	616	1/1	0.96	0.09	44,44,44,44	0
6	CL	C	613	1/1	0.96	0.11	32,32,32,32	0
6	CL	D	613	1/1	0.97	0.05	38,38,38,38	0
4	SO4	D	603	5/5	0.97	0.07	40,41,42,45	0
6	CL	B	610	1/1	0.97	0.14	46,46,46,46	0
6	CL	B	613	1/1	0.97	0.05	57,57,57,57	0
6	CL	C	610	1/1	0.97	0.05	32,32,32,32	0
4	SO4	B	603	5/5	0.98	0.08	26,29,30,32	0
4	SO4	A	602	5/5	0.98	0.06	37,38,38,41	0
6	CL	B	609	1/1	0.99	0.06	19,19,19,19	0

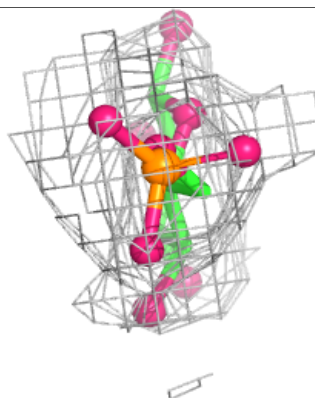
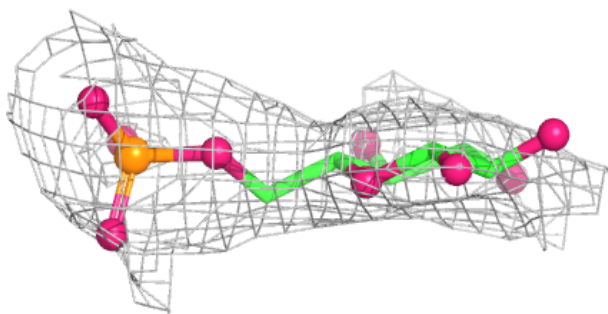
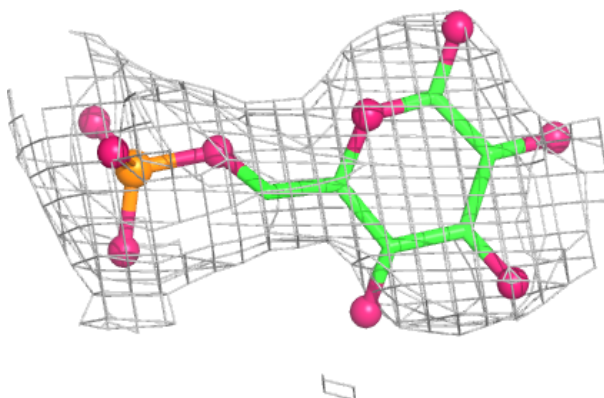
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BG6 C 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

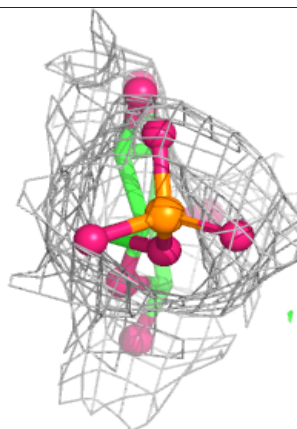
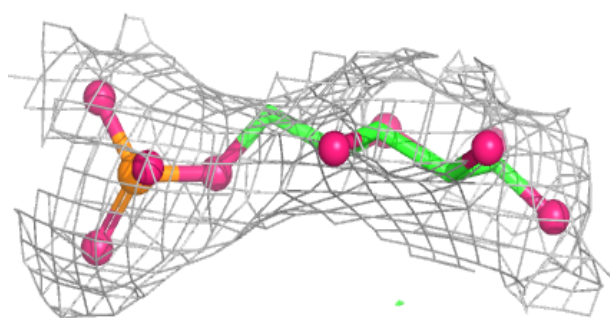
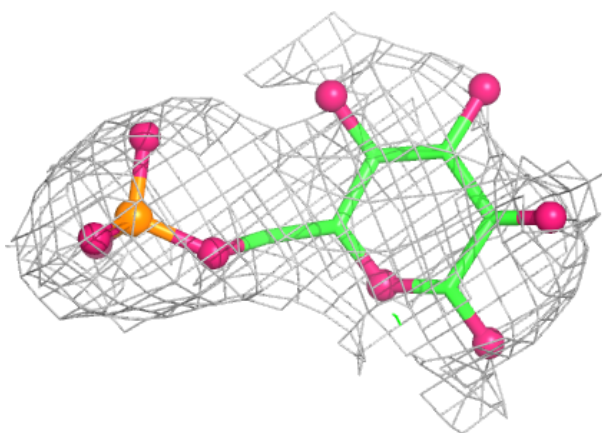
**Electron density around BG6 B 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

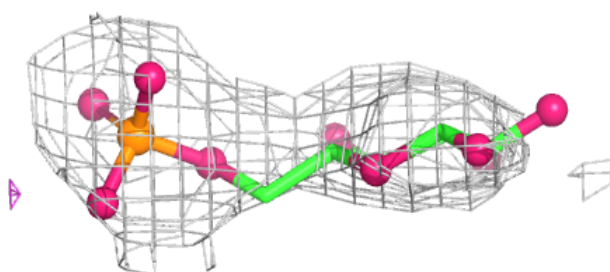
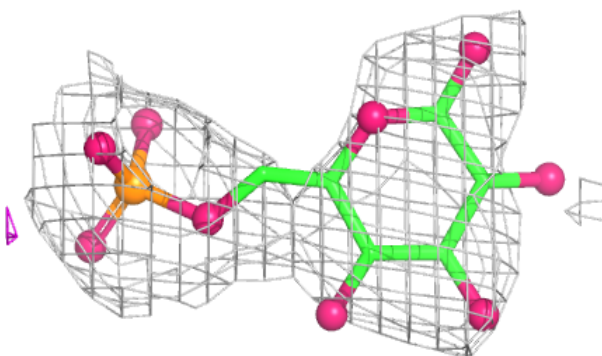


Electron density around BG6 D 602:

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

**Electron density around BG6 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.