



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:48 PM UTC

PDB ID : 1G0R / pdb_00001g0r
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). THYMIDINE/GLUCOSE-1-PHOSPHATE COMPLEX.
Authors : Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.
Deposited on : 2000-10-07
Resolution : 1.87 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

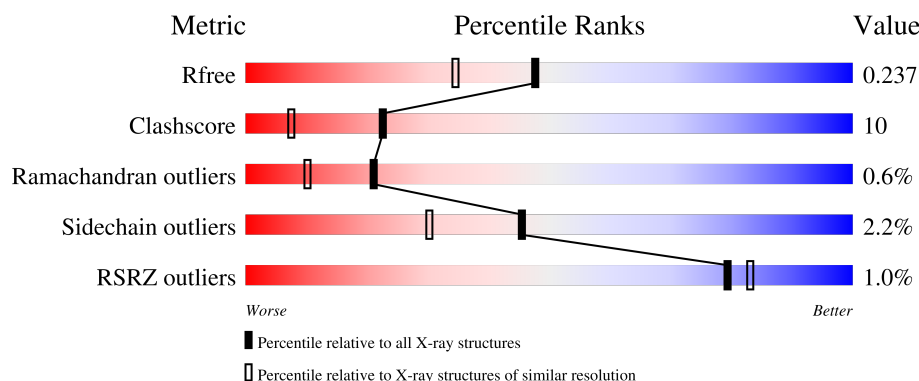
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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.



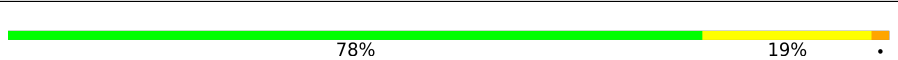
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	293	80% 18% .
1	B	293	74% 24% .
1	C	293	% 73% 22% 5%
1	D	293	2% 72% 23% ..

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Mol	Chain	Length	Quality of chain
1	E	293	
1	F	293	
1	G	293	
1	H	293	

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
3	SO4	A	2507	-	-	X	-
4	THM	F	2535	-	X	-	-

2 Entry composition

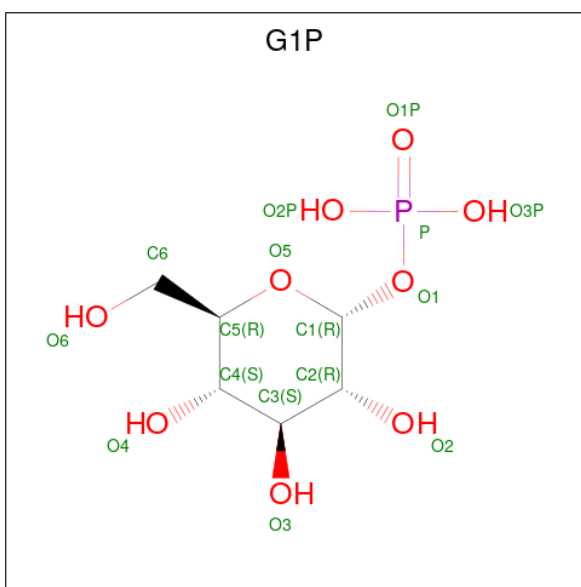
There are 5 unique types of molecules in this entry. The entry contains 21361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

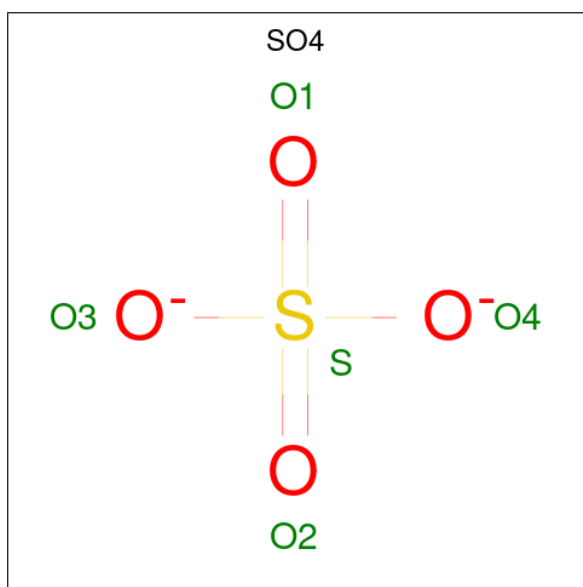
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	6	0
			2338	1493	396	444	5			
1	B	292	Total	C	N	O	S	0	8	0
			2350	1501	396	447	6			
1	C	292	Total	C	N	O	S	0	5	0
			2332	1491	395	441	5			
1	D	292	Total	C	N	O	S	0	5	0
			2325	1486	391	442	6			
1	E	292	Total	C	N	O	S	0	4	0
			2312	1477	389	440	6			
1	F	293	Total	C	N	O	S	0	5	0
			2340	1496	395	443	6			
1	G	292	Total	C	N	O	S	0	5	0
			2326	1487	390	443	6			
1	H	292	Total	C	N	O	S	0	2	0
			2303	1474	387	437	5			

- Molecule 2 is 1-O-phosphono-alpha-D-glucopyranose (CCD ID: G1P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		
2	E	1	Total	C	O	P	0	0
			16	6	9	1		
2	G	1	Total	C	O	P	0	0
			16	6	9	1		
2	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



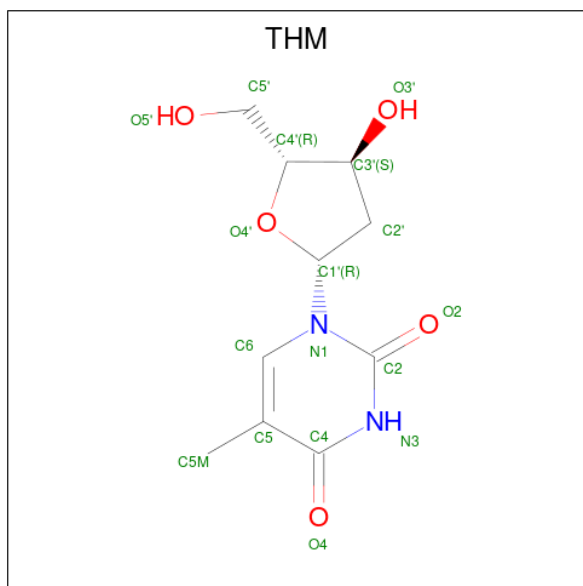
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is THYMIDINE (CCD ID: THM) (formula: C₁₀H₁₄N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	10	2	5		
4	A	1	Total	C	N	O	0	0
			17	10	2	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			17	10	2	5		
4	B	1	Total	C	N	O	0	0
			17	10	2	5		
4	C	1	Total	C	N	O	0	0
			17	10	2	5		
4	C	1	Total	C	N	O	0	0
			17	10	2	5		
4	D	1	Total	C	N	O	0	0
			17	10	2	5		
4	D	1	Total	C	N	O	0	0
			17	10	2	5		
4	E	1	Total	C	N	O	0	0
			17	10	2	5		
4	E	1	Total	C	N	O	0	0
			17	10	2	5		
4	F	1	Total	C	N	O	0	0
			17	10	2	5		
4	F	1	Total	C	N	O	0	0
			17	10	2	5		
4	G	1	Total	C	N	O	0	0
			17	10	2	5		
4	G	1	Total	C	N	O	0	0
			17	10	2	5		
4	H	1	Total	C	N	O	0	0
			17	10	2	5		
4	H	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	286	Total	O	0	0
			286	286		
5	B	307	Total	O	0	0
			307	307		
5	C	272	Total	O	0	0
			272	272		
5	D	266	Total	O	0	0
			266	266		
5	E	202	Total	O	0	0
			202	202		

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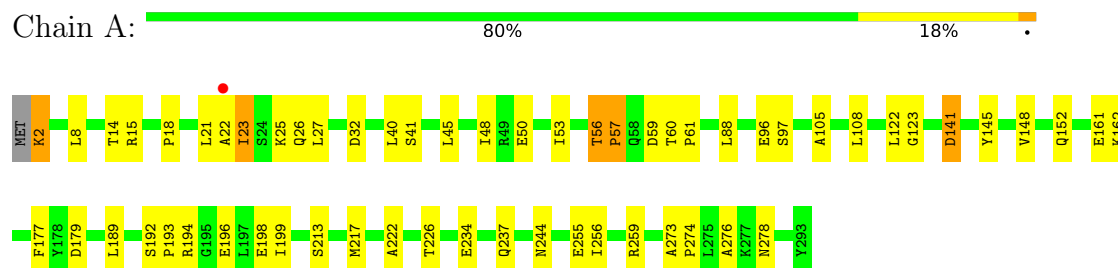
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	287	Total 287	O 287	0	0
5	G	327	Total 327	O 327	0	0
5	H	289	Total 289	O 289	0	0

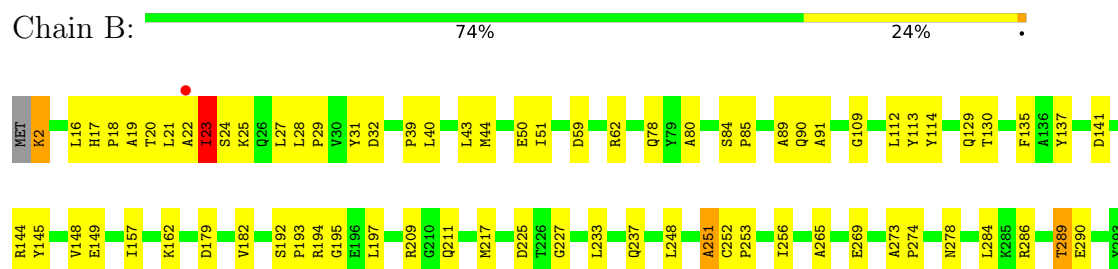
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

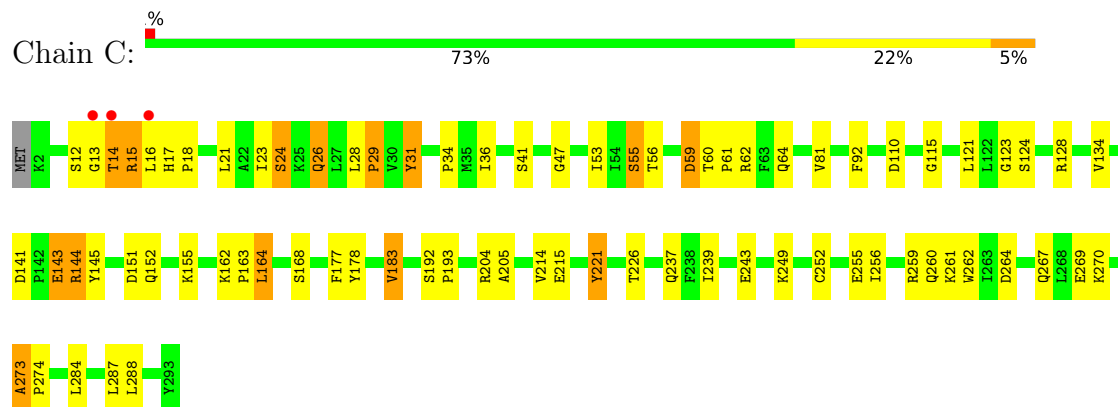
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

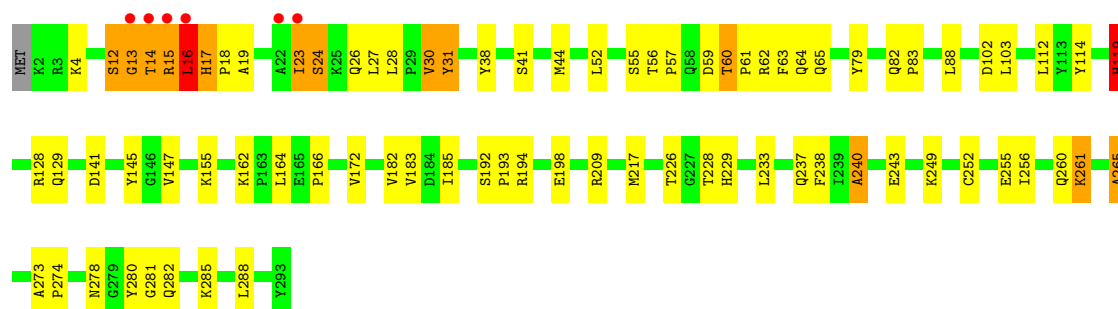


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

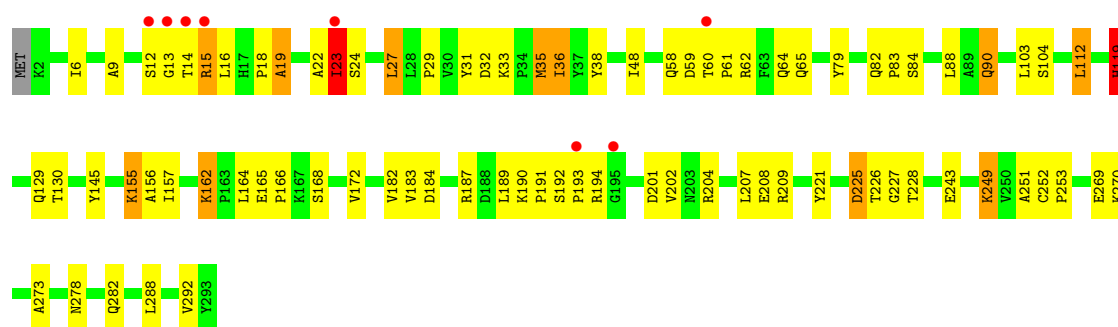


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE





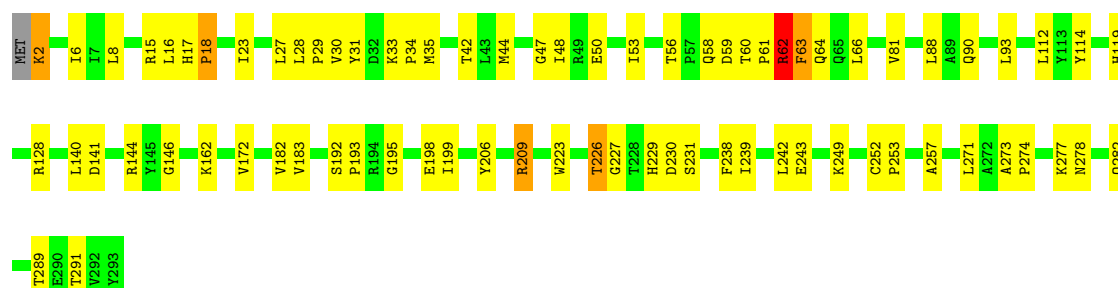
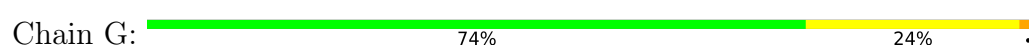
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



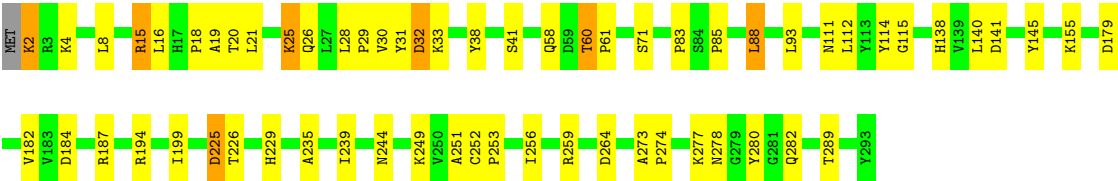
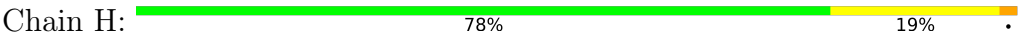
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



● Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.27Å 73.08Å 133.65Å 89.98° 81.42° 81.56°	Depositor
Resolution (Å)	73.00 – 1.87 73.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	84.0 (73.00-1.87) 84.7 (73.00-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.147 , 0.221 0.167 , 0.237	Depositor DCC
R_{free} test set	9145 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21361	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G1P, SO4, THM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.71	20/2389 (0.8%)	1.35	11/3241 (0.3%)
1	B	1.72	19/2401 (0.8%)	1.33	9/3256 (0.3%)
1	C	1.69	16/2383 (0.7%)	1.37	8/3232 (0.2%)
1	D	1.70	24/2375 (1.0%)	1.40	14/3222 (0.4%)
1	E	1.59	20/2362 (0.8%)	1.31	7/3205 (0.2%)
1	F	1.80	31/2391 (1.3%)	1.43	15/3242 (0.5%)
1	G	1.85	36/2377 (1.5%)	1.40	9/3225 (0.3%)
1	H	1.70	12/2354 (0.5%)	1.34	11/3195 (0.3%)
All	All	1.72	178/19032 (0.9%)	1.37	84/25818 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	E	0	1
All	All	0	3

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	162	LYS	C-O	-16.39	1.15	1.23
1	F	162	LYS	C-O	-9.94	1.19	1.23
1	G	44	MET	SD-CE	-9.59	1.55	1.79
1	A	217	MET	SD-CE	-9.25	1.56	1.79
1	B	44	MET	SD-CE	-8.75	1.57	1.79
1	B	217	MET	SD-CE	-8.71	1.57	1.79
1	A	162	LYS	C-O	-8.68	1.19	1.23
1	C	273	ALA	CA-CB	-8.29	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	62	ARG	C-O	-8.12	1.13	1.24
1	F	222	ALA	CA-CB	-8.09	1.41	1.53
1	D	30	VAL	CA-CB	-8.09	1.44	1.53
1	E	19	ALA	CA-CB	-8.09	1.40	1.53
1	A	23	ILE	CA-CB	-8.01	1.43	1.54
1	H	141	ASP	C-O	-7.98	1.15	1.24
1	G	30	VAL	CA-C	-7.98	1.44	1.52
1	C	239	ILE	CA-CB	-7.97	1.45	1.54
1	A	222	ALA	CA-CB	-7.76	1.43	1.53
1	C	214	VAL	C-O	-7.40	1.16	1.24
1	F	86	ASP	N-CA	-7.35	1.36	1.46
1	D	60	THR	C-O	-7.29	1.17	1.24
1	D	240	ALA	CA-C	-7.29	1.43	1.52
1	G	162	LYS	CA-CB	7.29	1.58	1.52
1	F	251	ALA	CA-CB	7.22	1.64	1.53
1	D	141	ASP	CA-C	7.22	1.61	1.53
1	C	28	LEU	C-O	-7.21	1.14	1.23
1	C	92	PHE	CA-C	7.20	1.62	1.52
1	E	9	ALA	CA-CB	-7.19	1.43	1.53
1	H	88	LEU	C-O	-7.19	1.15	1.24
1	B	23	ILE	CA-CB	-7.18	1.44	1.54
1	E	33	LYS	C-O	-7.17	1.16	1.24
1	G	289	THR	CA-CB	-7.17	1.43	1.53
1	D	217	MET	SD-CE	-6.96	1.62	1.79
1	D	15	ARG	N-CA	-6.95	1.37	1.46
1	A	53	ILE	CA-CB	-6.90	1.46	1.54
1	G	172	VAL	C-O	-6.88	1.15	1.24
1	G	81	VAL	C-O	-6.84	1.16	1.24
1	F	53	ILE	CA-CB	6.81	1.62	1.53
1	G	63	PHE	C-O	-6.71	1.16	1.24
1	B	157	ILE	CA-CB	6.64	1.63	1.54
1	A	177	PHE	CA-C	6.63	1.60	1.52
1	B	162	LYS	CA-CB	6.59	1.58	1.52
1	A	56	THR	CA-CB	6.57	1.62	1.53
1	G	231	SER	N-CA	-6.51	1.38	1.46
1	D	183	VAL	C-O	-6.50	1.16	1.24
1	G	56	THR	CA-CB	6.49	1.61	1.53
1	D	261	LYS	CA-C	6.44	1.61	1.53
1	H	235	ALA	CA-CB	-6.39	1.43	1.53
1	G	33	LYS	C-O	-6.36	1.17	1.24
1	D	114	TYR	CG-CD1	-6.35	1.26	1.39
1	E	172	VAL	C-O	-6.34	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	292	VAL	CA-CB	-6.33	1.45	1.53
1	A	105	ALA	CA-CB	-6.31	1.43	1.53
1	F	205	ALA	N-CA	-6.28	1.38	1.46
1	H	33	LYS	C-O	-6.27	1.18	1.24
1	F	182	VAL	CA-CB	-6.24	1.46	1.54
1	D	228	THR	CA-CB	-6.22	1.44	1.53
1	H	25	LYS	N-CA	-6.22	1.38	1.46
1	B	89	ALA	CA-CB	-6.21	1.42	1.53
1	G	42	THR	CA-C	-6.20	1.45	1.52
1	B	149	GLU	C-O	-6.19	1.16	1.23
1	D	162	LYS	CA-C	-6.12	1.49	1.53
1	F	2	LYS	C-O	6.10	1.31	1.23
1	C	168	SER	N-CA	-6.06	1.38	1.46
1	B	162	LYS	N-CA	6.04	1.50	1.46
1	H	239	ILE	CA-CB	-6.03	1.47	1.54
1	A	123	GLY	C-O	6.03	1.31	1.23
1	C	177	PHE	CA-C	6.02	1.59	1.52
1	D	265	ALA	CA-CB	6.02	1.62	1.53
1	E	155	LYS	CA-CB	6.00	1.62	1.53
1	G	34	PRO	CA-C	5.99	1.59	1.52
1	D	147	VAL	CA-CB	-5.98	1.47	1.54
1	E	35[A]	MET	SD-CE	-5.98	1.64	1.79
1	E	35[B]	MET	SD-CE	-5.98	1.64	1.79
1	G	90	GLN	C-O	-5.93	1.16	1.24
1	B	289	THR	CA-CB	-5.92	1.45	1.53
1	F	223	TRP	N-CA	-5.91	1.39	1.46
1	C	143	GLU	C-O	-5.91	1.16	1.24
1	G	230	ASP	C-O	-5.88	1.17	1.24
1	C	121	LEU	CA-C	5.87	1.60	1.52
1	F	198	GLU	CA-C	-5.86	1.45	1.52
1	A	226	THR	C-O	-5.81	1.14	1.23
1	F	112	LEU	N-CA	-5.81	1.39	1.46
1	F	222	ALA	CA-C	-5.80	1.45	1.52
1	B	40	LEU	C-O	5.79	1.30	1.24
1	C	47	GLY	C-O	-5.78	1.16	1.23
1	F	81	VAL	CB-CG1	-5.76	1.33	1.52
1	G	206	TYR	CA-C	5.75	1.60	1.52
1	E	6	ILE	N-CA	-5.73	1.39	1.46
1	G	48	ILE	CA-C	-5.73	1.45	1.52
1	H	239	ILE	N-CA	-5.68	1.39	1.46
1	F	168	SER	CA-C	-5.65	1.45	1.52
1	D	82	GLN	C-O	-5.64	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	273	ALA	CA-C	5.64	1.59	1.52
1	F	224	LEU	C-O	5.62	1.31	1.23
1	G	253	PRO	C-O	-5.60	1.17	1.24
1	F	217	MET	SD-CE	-5.60	1.65	1.79
1	F	110	ASP	C-O	-5.60	1.16	1.24
1	G	53	ILE	C-O	5.57	1.30	1.24
1	A	179	ASP	N-CA	-5.57	1.40	1.46
1	A	96	GLU	CA-C	5.56	1.60	1.52
1	F	254	GLU	C-O	-5.55	1.17	1.24
1	E	162	LYS	N-CA	5.55	1.50	1.46
1	D	44	MET	SD-CE	-5.55	1.65	1.79
1	E	166	PRO	C-O	-5.53	1.17	1.23
1	C	221	TYR	N-CA	-5.53	1.38	1.45
1	E	221	TYR	C-O	-5.50	1.17	1.23
1	B	91	ALA	C-O	5.49	1.30	1.24
1	G	140	LEU	N-CA	-5.48	1.39	1.46
1	G	128	ARG	CB-CG	-5.48	1.36	1.52
1	H	155	LYS	C-O	-5.45	1.17	1.24
1	F	2	LYS	N-CA	-5.44	1.39	1.46
1	E	90	GLN	C-O	-5.43	1.17	1.24
1	F	226	THR	N-CA	-5.42	1.40	1.46
1	C	134	VAL	N-CA	-5.41	1.39	1.46
1	A	189	LEU	CA-C	-5.39	1.45	1.52
1	G	257	ALA	C-O	-5.39	1.17	1.24
1	D	141	ASP	CA-CB	5.38	1.58	1.53
1	F	216	ILE	CA-C	-5.38	1.46	1.52
1	G	291	THR	CA-CB	-5.38	1.46	1.53
1	C	55	SER	CB-OG	5.38	1.52	1.42
1	G	58	GLN	CB-CG	-5.38	1.36	1.52
1	E	201	ASP	C-O	-5.36	1.17	1.24
1	F	76	ASP	C-O	-5.36	1.17	1.23
1	G	271	LEU	CG-CD2	-5.36	1.34	1.52
1	B	248	LEU	N-CA	-5.35	1.39	1.45
1	F	171	ALA	CA-C	-5.35	1.45	1.52
1	C	53	ILE	CG1-CD1	-5.33	1.30	1.51
1	G	183	VAL	C-O	5.33	1.30	1.24
1	D	255	GLU	C-O	-5.31	1.18	1.24
1	D	226	THR	C-O	-5.31	1.16	1.24
1	A	22	ALA	CA-C	5.29	1.59	1.52
1	F	234	GLU	CA-CB	5.28	1.61	1.53
1	F	107	VAL	CA-CB	-5.27	1.47	1.54
1	H	71	SER	C-O	-5.27	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	190	LYS	C-O	-5.27	1.17	1.24
1	F	180	GLN	CD-OE1	5.26	1.33	1.23
1	G	243	GLU	C-O	-5.26	1.17	1.24
1	D	15	ARG	CA-C	-5.26	1.45	1.52
1	A	21	LEU	CA-C	5.25	1.59	1.52
1	B	148	VAL	CA-CB	-5.24	1.48	1.54
1	B	78	GLN	N-CA	5.23	1.52	1.45
1	G	182	VAL	C-O	-5.23	1.18	1.24
1	D	172	VAL	C-O	-5.23	1.18	1.24
1	D	141	ASP	N-CA	5.23	1.52	1.46
1	H	244	ASN	N-CA	-5.23	1.39	1.46
1	A	213	SER	CA-C	5.22	1.59	1.52
1	F	200	THR	C-O	-5.21	1.18	1.24
1	D	155	LYS	C-O	-5.21	1.17	1.23
1	B	80	ALA	CA-CB	-5.19	1.44	1.54
1	G	6	ILE	N-CA	-5.19	1.40	1.46
1	E	112	LEU	CB-CG	-5.18	1.43	1.53
1	B	256	ILE	C-O	5.18	1.29	1.24
1	A	48	ILE	C-O	5.17	1.30	1.24
1	E	48	ILE	C-O	-5.17	1.18	1.24
1	E	38	TYR	N-CA	-5.17	1.42	1.46
1	G	50	GLU	C-O	5.17	1.30	1.24
1	G	223	TRP	CA-CB	5.16	1.61	1.53
1	H	20	THR	N-CA	5.14	1.52	1.46
1	A	234	GLU	C-O	-5.13	1.18	1.24
1	E	156	ALA	CA-CB	-5.13	1.45	1.53
1	A	148	VAL	C-O	-5.12	1.18	1.24
1	F	179	ASP	C-O	5.11	1.29	1.23
1	G	198	GLU	CA-CB	-5.10	1.45	1.53
1	D	238	PHE	N-CA	-5.10	1.40	1.46
1	B	137	TYR	C-O	5.07	1.29	1.24
1	C	183	VAL	CA-CB	-5.07	1.48	1.54
1	F	134	VAL	N-CA	-5.07	1.40	1.46
1	B	135	PHE	C-O	5.06	1.30	1.24
1	C	36	ILE	C-O	-5.06	1.17	1.24
1	D	243	GLU	C-O	-5.06	1.18	1.24
1	E	36	ILE	CG1-CD1	-5.06	1.32	1.51
1	G	195	GLY	CA-C	5.06	1.58	1.51
1	H	138	HIS	CA-CB	-5.05	1.45	1.53
1	A	57	PRO	C-O	-5.03	1.17	1.24
1	B	265	ALA	CA-CB	5.02	1.61	1.53
1	G	64	GLN	C-O	-5.02	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	101	ASN	N-CA	-5.01	1.40	1.46
1	G	47	GLY	C-O	-5.01	1.17	1.24

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	GLY	N-CA-C	-10.53	101.11	114.37
1	H	20	THR	N-CA-C	9.84	125.02	112.92
1	A	21	LEU	N-CA-C	-9.19	101.17	111.82
1	D	185	ILE	N-CA-C	-8.03	102.72	110.42
1	D	13	GLY	CA-C-O	7.23	126.57	119.27
1	F	11	GLY	N-CA-C	-7.12	103.72	112.33
1	F	162	LYS	CB-CA-C	-6.84	106.34	111.20
1	F	129	GLN	CA-CB-CG	-6.84	100.42	114.10
1	G	66	LEU	N-CA-C	6.81	118.36	111.07
1	F	41	SER	CA-CB-OG	-6.76	97.58	111.10
1	F	81	VAL	N-CA-C	6.64	118.35	108.46
1	D	217	MET	CA-C-N	6.60	127.63	120.44
1	D	217	MET	C-N-CA	6.60	127.63	120.44
1	H	182	VAL	N-CA-C	6.54	117.33	110.72
1	B	17	HIS	N-CA-C	6.44	117.01	109.60
1	F	24	SER	N-CA-CB	-6.42	99.48	109.69
1	B	227	GLY	N-CA-C	6.34	121.65	114.67
1	D	23	ILE	N-CA-C	6.33	116.74	107.75
1	B	182	VAL	N-CA-C	6.25	116.42	110.42
1	F	118	PHE	N-CA-C	-6.12	104.68	111.36
1	E	104	SER	N-CA-C	6.09	118.04	108.96
1	G	93	LEU	N-CA-C	-6.06	103.32	112.04
1	A	23	ILE	N-CA-CB	-6.04	101.26	111.23
1	G	209	ARG	NE-CZ-NH2	-6.02	113.78	119.20
1	B	251	ALA	N-CA-C	6.02	119.76	111.63
1	H	226	THR	OG1-CB-CG2	-5.99	97.31	109.30
1	A	40	LEU	N-CA-C	-5.97	104.68	111.07
1	B	21	LEU	N-CA-C	-5.93	104.94	111.82
1	G	239	ILE	N-CA-C	-5.90	104.76	110.72
1	C	59	ASP	N-CA-C	5.84	120.14	112.89
1	C	205	ALA	N-CA-C	-5.83	105.00	111.36
1	C	21	LEU	N-CA-C	-5.81	104.91	112.23
1	D	182	VAL	N-CA-C	5.80	116.54	110.62
1	A	122	LEU	CA-C-N	5.80	126.42	119.98
1	A	122	LEU	C-N-CA	5.80	126.42	119.98
1	A	276	ALA	N-CA-C	5.78	118.36	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	PRO	CB-CA-C	-5.75	102.74	110.85
1	A	141	ASP	CA-C-N	5.73	125.59	119.28
1	A	141	ASP	C-N-CA	5.73	125.59	119.28
1	A	97	SER	N-CA-CB	5.71	118.51	110.12
1	G	227	GLY	N-CA-C	5.67	121.03	114.16
1	D	55	SER	N-CA-C	5.60	115.51	108.45
1	B	109	GLY	N-CA-C	5.58	120.55	113.24
1	E	182	VAL	N-CA-C	5.55	115.75	110.42
1	A	45	LEU	N-CA-C	-5.50	106.06	112.89
1	G	226	THR	N-CA-C	5.49	118.77	112.57
1	G	18	PRO	CB-CG-CD	5.46	117.96	105.40
1	D	15	ARG	N-CA-CB	-5.41	101.34	110.49
1	H	115	GLY	N-CA-C	5.40	118.15	111.19
1	H	58	GLN	N-CA-C	5.36	117.20	111.36
1	H	280	TYR	N-CA-C	-5.35	105.36	111.14
1	B	43	LEU	N-CA-C	5.35	116.80	111.07
1	H	93	LEU	N-CA-C	-5.33	105.05	112.45
1	E	282	GLN	N-CA-C	-5.32	105.39	111.14
1	F	20	THR	N-CA-C	5.32	118.89	112.93
1	F	157	ILE	N-CA-C	5.32	118.74	113.53
1	D	119	HIS	N-CA-CB	-5.30	102.33	110.12
1	F	198	GLU	CB-CA-C	-5.29	101.13	109.80
1	C	29	PRO	CB-CA-C	-5.27	104.07	110.98
1	C	288	LEU	N-CA-C	5.27	117.93	111.82
1	F	157	ILE	CB-CA-C	-5.26	105.50	110.65
1	D	217	MET	N-CA-C	-5.25	99.21	108.20
1	H	60	THR	CA-C-O	5.25	123.43	118.34
1	D	128	ARG	CB-CA-C	5.24	119.52	110.77
1	A	198	GLU	N-CA-C	5.23	118.14	109.46
1	H	32	ASP	N-CA-C	5.21	121.36	114.12
1	G	242	LEU	N-CA-C	5.20	116.64	111.07
1	E	23	ILE	N-CA-C	5.19	115.84	108.42
1	H	140	LEU	CA-C-N	-5.18	116.66	123.34
1	H	140	LEU	C-N-CA	-5.18	116.66	123.34
1	B	39	PRO	N-CD-CG	5.14	110.92	103.20
1	F	239	ILE	N-CA-C	5.14	115.36	110.42
1	E	157	ILE	N-CA-C	5.13	118.56	113.53
1	C	178	TYR	N-CA-C	5.13	117.61	109.50
1	F	67	LEU	N-CA-C	5.13	119.81	113.50
1	D	52	LEU	N-CA-C	5.10	117.04	108.73
1	E	249	LYS	CB-CA-C	5.09	118.69	109.37
1	G	146	GLY	N-CA-C	-5.07	103.93	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	PRO	CA-C-O	-5.05	115.58	121.34
1	E	162	LYS	CB-CA-C	-5.02	107.64	111.20
1	D	166	PRO	CA-C-O	-5.02	115.55	121.67
1	C	144	ARG	N-CA-C	5.01	119.37	113.16
1	F	217	MET	CA-C-N	5.00	125.89	120.44
1	F	217	MET	C-N-CA	5.00	125.89	120.44

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	119	HIS	Sidechain
1	D	16	LEU	Peptide
1	E	119	HIS	Sidechain

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	2338	0	2315	37	0
1	B	2350	0	2327	50	0
1	C	2332	0	2315	66	0
1	D	2325	0	2307	65	0
1	E	2312	0	2295	69	0
1	F	2340	0	2326	55	0
1	G	2326	0	2303	38	0
1	H	2303	0	2285	46	0
2	A	16	0	11	2	0
2	B	16	0	11	2	0
2	C	16	0	11	2	0
2	D	16	0	11	2	0
2	E	16	0	11	3	0
2	G	16	0	11	1	0
2	H	16	0	11	1	0
3	A	10	0	0	3	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	20	0	0	0	0
3	E	10	0	0	1	0
3	F	20	0	0	1	0
3	G	10	0	0	0	0
3	H	15	0	0	2	0
4	A	34	0	27	1	0
4	B	34	0	27	0	0
4	C	34	0	27	0	0
4	D	34	0	27	0	0
4	E	34	0	27	0	0
4	F	34	0	26	2	0
4	G	34	0	27	1	0
4	H	34	0	27	2	0
5	A	286	0	0	4	0
5	B	307	0	0	12	0
5	C	272	0	0	17	0
5	D	266	0	0	15	0
5	E	202	0	0	15	0
5	F	287	0	0	19	0
5	G	327	0	0	10	0
5	H	289	0	0	15	0
All	All	21361	0	18765	397	0

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

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASP:HB2	5:B:2787:HOH:O	1.33	1.25
1:G:282:GLN:HG2	5:G:2851:HOH:O	1.38	1.23
1:G:141:ASP:HB2	5:G:2617:HOH:O	1.39	1.18
1:H:60:THR:HG23	5:H:2715:HOH:O	1.51	1.10
5:B:2699:HOH:O	1:E:155:LYS:HE3	1.63	0.99
1:C:60:THR:HG23	5:C:2621:HOH:O	1.63	0.98
1:C:26:GLN:H	1:C:26:GLN:HE21	1.03	0.97
1:B:145:TYR:HD2	2:B:2501:G1P:H5	1.32	0.93
1:C:31:TYR:CD1	1:D:233[B]:LEU:HD11	2.04	0.92
1:C:31:TYR:HD1	1:D:233[B]:LEU:HD11	1.33	0.92
1:F:215:GLU:HG2	5:F:2819:HOH:O	1.69	0.90
1:C:26:GLN:H	1:C:26:GLN:NE2	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:HG2	5:B:2838:HOH:O	1.70	0.89
1:E:23:ILE:HG21	1:F:23:ILE:HG12	1.57	0.86
1:E:190:LYS:HD2	1:E:191:PRO:HD2	1.56	0.86
1:F:14:THR:HA	1:F:17:HIS:ND1	1.90	0.85
1:C:13:GLY:O	1:C:17:HIS:CD2	2.29	0.84
1:F:119:HIS:CE1	1:F:120:GLU:OE1	2.31	0.84
1:C:26:GLN:HE21	1:C:26:GLN:N	1.77	0.83
1:C:60:THR:HG22	1:C:64:GLN:HE21	1.44	0.83
1:C:155:LYS:HD2	5:C:2664:HOH:O	1.78	0.82
1:A:2:LYS:NZ	1:A:50:GLU:OE1	2.10	0.81
1:D:65:GLN:HG3	5:D:2631:HOH:O	1.82	0.79
1:C:15:ARG:HG2	1:C:16:LEU:HD23	1.62	0.79
1:B:23:ILE:HG12	1:B:27:LEU:HD12	1.64	0.78
1:A:237[B]:GLN:HE22	1:B:237[B]:GLN:HE21	1.28	0.78
1:D:15:ARG:HG2	5:D:2632:HOH:O	1.83	0.78
1:F:273:ALA:HB3	1:F:274:PRO:HD3	1.66	0.77
1:F:23:ILE:HA	5:F:2607:HOH:O	1.83	0.77
1:B:145:TYR:CD2	2:B:2501:G1P:H5	2.17	0.77
1:F:119:HIS:NE2	1:F:120:GLU:OE1	2.17	0.77
5:E:2600:HOH:O	1:F:62:ARG:HG2	1.85	0.76
1:C:270:LYS:NZ	5:C:2679:HOH:O	2.19	0.76
1:A:141:ASP:HB2	5:A:2637:HOH:O	1.84	0.75
1:F:16:LEU:O	1:F:19:ALA:HB3	1.87	0.75
1:F:215:GLU:HG3	5:F:2748:HOH:O	1.87	0.75
1:H:229:HIS:HD2	5:H:2748:HOH:O	1.70	0.75
3:A:2507:SO4:O2	5:A:2824:HOH:O	2.05	0.74
1:A:237[A]:GLN:HG2	1:C:237[A]:GLN:HG2	1.70	0.74
1:B:2:LYS:N	5:B:2749:HOH:O	2.21	0.74
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.70	0.73
1:A:237[B]:GLN:HG3	1:B:233:LEU:HD11	1.70	0.73
1:F:57:PRO:HG3	1:F:81:VAL:HG11	1.71	0.73
1:C:124:SER:HB2	5:C:2763:HOH:O	1.89	0.73
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.52	0.72
1:C:141:ASP:HB3	5:C:2645:HOH:O	1.89	0.72
1:D:12:SER:HB3	1:D:14:THR:OG1	1.90	0.72
1:E:27:LEU:HB2	1:F:23:ILE:HD11	1.71	0.72
1:F:14:THR:HA	1:F:17:HIS:CE1	2.23	0.72
1:F:62:ARG:NH2	5:F:2760:HOH:O	2.22	0.71
1:C:155:LYS:HE3	5:C:2688:HOH:O	1.90	0.71
1:A:14:THR:N	3:A:2507:SO4:O1	2.22	0.71
1:C:256:ILE:O	1:C:260:GLN:HG3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:TYR:CD1	1:D:233[B]:LEU:CD1	2.74	0.70
1:H:259:ARG:NH1	5:H:2568:HOH:O	2.23	0.69
1:C:23:ILE:HD13	1:D:23:ILE:HG21	1.74	0.69
1:B:22:ALA:O	1:B:23:ILE:HB	1.92	0.69
3:H:2518:SO4:O2	5:H:2671:HOH:O	2.11	0.69
1:C:264:ASP:OD1	1:C:267:GLN:HG3	1.93	0.68
1:C:260:GLN:O	1:C:261:LYS:HB2	1.93	0.68
1:D:14:THR:O	1:D:17:HIS:ND1	2.26	0.68
1:C:31:TYR:HD1	1:D:233[B]:LEU:CD1	2.05	0.68
1:G:28:LEU:HD22	1:H:29:PRO:HD3	1.76	0.68
1:E:24:SER:HB3	1:E:27:LEU:HD12	1.76	0.68
1:F:119:HIS:NE2	1:F:120:GLU:CD	2.52	0.68
1:C:152:GLN:NE2	5:C:2779:HOH:O	2.27	0.67
1:C:269:GLU:HG3	5:C:2691:HOH:O	1.94	0.66
1:A:237[B]:GLN:CG	1:B:233:LEU:HD11	2.24	0.66
1:E:23:ILE:HG21	1:F:23:ILE:CG1	2.24	0.66
1:G:2:LYS:N	5:G:2744:HOH:O	2.28	0.66
1:H:145:TYR:HD2	2:H:2506:G1P:H5	1.60	0.66
1:E:16:LEU:O	1:E:19:ALA:HB3	1.95	0.65
1:D:112:LEU:C	1:D:112:LEU:HD23	2.21	0.65
1:E:112:LEU:C	1:E:112:LEU:HD23	2.22	0.64
1:H:85:PRO:O	5:H:2780:HOH:O	2.14	0.64
1:B:59:ASP:OD1	1:B:62:ARG:NH1	2.30	0.64
1:E:22:ALA:C	1:E:23:ILE:HG13	2.23	0.64
1:E:65:GLN:OE1	5:E:2742:HOH:O	2.15	0.63
1:E:187:ARG:NH2	5:E:2622:HOH:O	2.31	0.63
1:E:60:THR:HB	1:E:61:PRO:HD3	1.80	0.63
1:A:255:GLU:O	1:A:259[B]:ARG:HG3	1.99	0.63
1:C:269:GLU:CD	5:C:2715:HOH:O	2.41	0.63
1:B:114[B]:TYR:C	1:B:114[B]:TYR:CD2	2.76	0.62
1:F:244:ASN:ND2	5:F:2663:HOH:O	2.32	0.62
1:D:15:ARG:O	1:D:17:HIS:HB2	2.00	0.62
5:B:2815:HOH:O	1:E:209:ARG:NE	2.31	0.61
1:E:16:LEU:HD21	1:E:228:THR:HA	1.82	0.61
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.64	0.61
1:G:192:SER:HB2	1:G:193:PRO:CD	2.31	0.61
1:C:144:ARG:HG3	5:C:2645:HOH:O	1.99	0.61
1:D:23:ILE:HD11	1:D:27:LEU:HD13	1.83	0.61
1:E:22:ALA:HA	5:F:2768:HOH:O	2.01	0.61
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.84	0.60
1:D:192:SER:HB2	1:D:193:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ARG:HD2	5:E:2717:HOH:O	2.01	0.60
1:G:27:LEU:HG	1:G:63:PHE:CE2	2.34	0.60
1:C:23:ILE:CD1	1:D:23:ILE:HG21	2.32	0.60
1:D:282:GLN:HG2	5:D:2794:HOH:O	2.01	0.60
1:D:12:SER:CB	1:D:14:THR:OG1	2.48	0.60
1:E:103:LEU:HD11	1:E:129:GLN:HG2	1.84	0.60
1:D:233[B]:LEU:O	1:D:237[B]:GLN:HG3	2.01	0.60
1:G:273:ALA:HB3	1:G:274:PRO:CD	2.31	0.60
1:E:65:GLN:HB2	5:E:2720:HOH:O	2.02	0.60
1:D:59:ASP:HA	1:D:62:ARG:HD2	1.84	0.59
1:D:88:LEU:HD11	2:D:2503:G1P:H1	1.84	0.59
1:A:244:ASN:HB3	5:A:2685:HOH:O	2.00	0.59
1:H:264:ASP:C	1:H:264:ASP:OD1	2.45	0.59
1:C:128:ARG:NH1	1:C:215:GLU:OE2	2.34	0.59
1:E:60:THR:HB	1:E:61:PRO:CD	2.32	0.59
1:C:26:GLN:NE2	1:C:26:GLN:N	2.44	0.58
4:F:2535:THM:H2'2	4:F:2535:THM:O5'	2.03	0.58
3:H:2526:SO4:O4	5:H:2826:HOH:O	2.15	0.58
1:E:61:PRO:HB2	5:E:2732:HOH:O	2.04	0.58
1:E:190:LYS:HD2	1:E:191:PRO:CD	2.30	0.58
1:A:23:ILE:HD11	1:A:27:LEU:HD13	1.85	0.58
1:B:144:ARG:HD3	5:B:2787:HOH:O	2.04	0.58
1:F:141:ASP:OD2	1:F:144:ARG:NH2	2.31	0.58
1:H:60:THR:N	1:H:61:PRO:CD	2.67	0.58
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.86	0.58
1:E:192:SER:HB2	1:E:193:PRO:CD	2.34	0.58
1:B:23:ILE:HD11	1:B:62:ARG:HD3	1.86	0.57
1:A:278:ASN:HB2	5:B:2680:HOH:O	2.02	0.57
1:D:24:SER:HB2	5:D:2591:HOH:O	2.04	0.57
1:A:18:PRO:HD2	1:B:32:ASP:O	2.04	0.57
1:E:64:GLN:HA	1:E:79:TYR:CZ	2.40	0.57
1:E:23:ILE:HG21	1:F:23:ILE:CD1	2.34	0.57
1:B:289:THR:HG23	5:B:2671:HOH:O	2.04	0.57
1:G:249:LYS:HB2	1:G:252[B]:CYS:SG	2.44	0.57
1:E:130[A]:THR:HG22	3:E:2520:SO4:O2	2.05	0.56
1:F:192:SER:HB2	1:F:193:PRO:HD2	1.87	0.56
1:B:112:LEU:HD23	1:B:112:LEU:C	2.30	0.56
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.87	0.56
1:G:16:LEU:O	1:G:17:HIS:C	2.48	0.56
1:G:144:ARG:HD3	5:G:2617:HOH:O	2.05	0.56
1:C:41:SER:HB2	1:C:256:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:LEU:HD13	5:F:2729:HOH:O	2.04	0.56
1:C:24:SER:HB3	1:C:59:ASP:OD2	2.06	0.56
1:D:16:LEU:HD22	1:D:229:HIS:CD2	2.41	0.56
1:E:162:LYS:NZ	2:E:2504:G1P:O3P	2.26	0.56
1:H:60:THR:HB	1:H:61:PRO:HD3	1.87	0.56
1:B:289:THR:CG2	5:B:2671:HOH:O	2.53	0.56
1:H:15:ARG:NH1	5:H:2826:HOH:O	2.39	0.56
1:B:23:ILE:HD11	1:B:27:LEU:HD13	1.88	0.55
1:G:119:HIS:CD2	5:G:2791:HOH:O	2.59	0.55
1:F:23:ILE:HG23	5:F:2607:HOH:O	2.05	0.55
1:E:32:ASP:OD2	1:E:243:GLU:OE1	2.24	0.55
1:H:2:LYS:HE2	1:H:4:LYS:HG3	1.87	0.55
1:E:23:ILE:HG22	1:E:27:LEU:HD13	1.89	0.55
1:B:23:ILE:CG1	1:B:27:LEU:HD12	2.37	0.54
1:G:192:SER:HB2	1:G:193:PRO:HD2	1.89	0.54
5:C:2590:HOH:O	1:D:233[B]:LEU:HD23	2.07	0.54
1:H:8:LEU:HG	4:H:2537:THM:O2	2.08	0.54
1:E:59:ASP:O	1:E:60:THR:C	2.50	0.54
1:F:209:ARG:CD	5:F:2802:HOH:O	2.55	0.54
1:G:273:ALA:N	1:G:274:PRO:HD2	2.22	0.54
1:H:41:SER:HB2	1:H:256:ILE:CD1	2.38	0.54
1:F:141:ASP:CG	1:F:144:ARG:HH21	2.14	0.54
1:F:287:LEU:HG	5:F:2746:HOH:O	2.07	0.54
1:C:164:LEU:HB3	5:C:2752:HOH:O	2.08	0.54
1:H:30:VAL:HB	1:H:38:TYR:CE1	2.43	0.53
1:E:27:LEU:CB	1:F:23:ILE:HD11	2.39	0.53
1:F:238:PHE:CE1	1:G:238:PHE:CE1	2.97	0.53
1:C:14:THR:HA	1:C:17:HIS:ND1	2.24	0.53
1:D:260:GLN:O	1:D:261:LYS:HB2	2.09	0.53
1:E:145:TYR:HD2	2:E:2504:G1P:H5	1.74	0.53
1:A:192:SER:HB2	1:A:193:PRO:CD	2.37	0.53
1:C:24:SER:CB	1:C:59:ASP:OD2	2.57	0.53
1:D:103:LEU:HD11	1:D:129:GLN:HG2	1.92	0.52
1:B:23:ILE:CG1	1:B:24:SER:H	2.21	0.52
1:G:28:LEU:HD22	1:H:29:PRO:CD	2.40	0.52
1:A:32:ASP:O	1:B:18:PRO:HD2	2.10	0.52
1:C:60:THR:HG22	1:C:64:GLN:NE2	2.20	0.52
1:H:25:LYS:HE3	1:H:26:GLN:HE22	1.74	0.52
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.91	0.52
1:F:209:ARG:HD3	5:F:2802:HOH:O	2.09	0.52
1:H:194:ARG:HG3	5:H:2816:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:ALA:HB3	1:H:274:PRO:CD	2.40	0.51
1:C:14:THR:O	1:D:278:ASN:ND2	2.43	0.51
1:E:192:SER:HB2	1:E:193:PRO:HD2	1.93	0.51
1:F:16:LEU:HD22	5:F:2729:HOH:O	2.08	0.51
1:G:88:LEU:HD11	2:G:2505:G1P:H1	1.92	0.51
1:A:88:LEU:HD13	1:A:108:LEU:HD21	1.92	0.51
1:A:88:LEU:HD11	2:A:2500:G1P:H1	1.92	0.51
1:D:24:SER:HB3	1:D:59:ASP:CG	2.35	0.51
1:H:16:LEU:O	1:H:19:ALA:HB3	2.10	0.51
1:H:251:ALA:O	1:H:253:PRO:HD3	2.10	0.51
1:C:13:GLY:O	1:C:17:HIS:NE2	2.44	0.51
1:D:83:PRO:HD2	5:D:2659:HOH:O	2.10	0.51
1:E:225:ASP:C	1:E:225:ASP:OD1	2.54	0.51
1:D:249:LYS:HB2	1:D:252[B]:CYS:SG	2.51	0.51
1:C:260:GLN:O	1:C:261:LYS:CB	2.58	0.51
1:E:58:GLN:HB2	5:E:2598:HOH:O	2.10	0.51
1:F:124:SER:HB2	5:F:2575:HOH:O	2.10	0.51
1:G:8:LEU:HD21	1:G:88:LEU:HA	1.92	0.51
1:G:141:ASP:OD1	5:G:2681:HOH:O	2.19	0.51
1:B:23:ILE:CD1	1:B:62:ARG:HD3	2.41	0.51
1:F:273:ALA:HB3	1:F:274:PRO:CD	2.39	0.51
1:G:273:ALA:HB3	1:G:274:PRO:HD3	1.92	0.51
4:G:2536:THM:H5'2	5:G:2685:HOH:O	2.10	0.50
1:A:145:TYR:HD2	2:A:2500:G1P:H5	1.76	0.50
1:E:88:LEU:HD11	2:E:2504:G1P:H1	1.94	0.50
1:B:2:LYS:CA	5:B:2749:HOH:O	2.59	0.50
1:C:110:ASP:HB2	1:C:226:THR:OG1	2.11	0.50
1:E:29:PRO:HG3	5:E:2649:HOH:O	2.12	0.50
1:F:4[B]:LYS:HE3	1:F:50:GLU:CD	2.37	0.50
1:G:29:PRO:HD3	1:H:28:LEU:HD22	1.94	0.50
1:G:229:HIS:HB3	1:H:31:TYR:CE1	2.47	0.50
1:D:56:THR:HB	1:D:57:PRO:HD2	1.93	0.49
1:B:90:GLN:HG2	1:B:197:LEU:HD12	1.94	0.49
1:H:114[B]:TYR:C	1:H:114[B]:TYR:CD2	2.90	0.49
1:C:23:ILE:HG12	1:D:23:ILE:HD13	1.94	0.49
1:C:243:GLU:HG2	1:C:249:LYS:HA	1.95	0.49
4:F:2535:THM:O5'	4:F:2535:THM:H6	2.12	0.49
1:C:145:TYR:HD2	2:C:2502:G1P:H5	1.77	0.49
1:H:18:PRO:O	1:H:19:ALA:C	2.54	0.49
1:B:112:LEU:HD23	1:B:113:TYR:N	2.28	0.49
1:H:8:LEU:HG	4:H:2537:THM:C2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HE3	1:A:26:GLN:HE22	1.78	0.49
1:C:260:GLN:CG	5:C:2751:HOH:O	2.61	0.49
1:E:278:ASN:ND2	1:F:14:THR:O	2.46	0.49
1:A:8:LEU:HG	4:A:2530:THM:O2	2.13	0.48
1:C:143:GLU:OE2	5:C:2645:HOH:O	2.20	0.48
1:D:56:THR:O	1:D:60:THR:OG1	2.31	0.48
1:B:23:ILE:CG1	1:B:24:SER:N	2.76	0.48
1:C:162:LYS:NZ	2:C:2502:G1P:O3P	2.46	0.48
1:F:152:GLN:HG2	3:F:2524:SO4:O3	2.13	0.48
1:H:229:HIS:NE2	5:H:2678:HOH:O	2.35	0.48
1:C:260:GLN:CD	5:C:2751:HOH:O	2.55	0.48
1:C:14:THR:HA	1:C:17:HIS:CE1	2.48	0.48
1:H:83:PRO:HD2	5:H:2691:HOH:O	2.14	0.48
1:A:237[B]:GLN:NE2	1:B:237[B]:GLN:HE21	2.04	0.48
1:B:251:ALA:O	1:B:253:PRO:HD3	2.13	0.48
1:G:18:PRO:HD2	1:H:32:ASP:O	2.14	0.48
1:H:249:LYS:HB3	1:H:252[B]:CYS:SG	2.54	0.48
1:C:59:ASP:OD1	1:C:62:ARG:NH1	2.40	0.48
1:D:16:LEU:HA	5:D:2632:HOH:O	2.14	0.47
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.43	0.47
1:F:21:LEU:HD23	1:F:21:LEU:HA	1.51	0.47
1:F:215:GLU:CG	5:F:2748:HOH:O	2.53	0.47
1:C:192:SER:HB2	1:C:193:PRO:CD	2.45	0.47
1:E:24:SER:HB3	1:E:27:LEU:CD1	2.43	0.47
1:A:41:SER:HB2	1:A:256:ILE:CD1	2.45	0.47
1:G:23:ILE:CD1	1:H:28:LEU:HD23	2.44	0.47
1:C:13:GLY:O	1:C:17:HIS:CG	2.67	0.47
1:E:59:ASP:O	1:E:62:ARG:N	2.35	0.47
1:E:59:ASP:O	1:E:62:ARG:HB2	2.14	0.47
1:E:60:THR:CB	1:E:61:PRO:CD	2.92	0.47
1:G:249:LYS:CB	1:G:252[B]:CYS:SG	3.02	0.47
1:H:249:LYS:CB	1:H:252[B]:CYS:SG	3.03	0.47
1:D:4:LYS:HE3	1:D:102:ASP:OD2	2.14	0.47
1:F:24:SER:OG	1:F:59:ASP:OD2	2.18	0.47
1:F:57:PRO:HG3	1:F:81:VAL:CG1	2.44	0.47
1:G:114[B]:TYR:CD2	1:G:114[B]:TYR:C	2.93	0.46
1:A:152:GLN:HG2	5:A:2576:HOH:O	2.14	0.46
1:D:13:GLY:HA2	5:D:2566:HOH:O	2.15	0.46
1:E:24:SER:HB2	1:E:59:ASP:OD2	2.16	0.46
1:G:277:LYS:NZ	5:G:2814:HOH:O	2.48	0.46
1:B:84:SER:OG	1:B:85:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:GLN:O	1:F:286:ARG:HG3	2.15	0.46
1:H:225:ASP:OD1	1:H:225:ASP:C	2.58	0.46
1:E:18:PRO:O	1:E:19:ALA:C	2.57	0.46
1:E:24:SER:CB	1:E:27:LEU:HD12	2.46	0.46
1:H:8:LEU:HD23	1:H:88:LEU:HD22	1.97	0.46
1:A:15:ARG:HG2	5:B:2827:HOH:O	2.15	0.46
1:E:22:ALA:CB	5:F:2768:HOH:O	2.63	0.46
1:B:252[B]:CYS:SG	1:B:284:LEU:HD21	2.56	0.45
1:A:56:THR:HB	1:A:57:PRO:HD2	1.97	0.45
1:E:183:VAL:O	1:E:187:ARG:HG3	2.16	0.45
1:H:21:LEU:N	5:H:2639:HOH:O	2.49	0.45
1:H:273:ALA:HB3	1:H:274:PRO:HD3	1.98	0.45
1:A:60:THR:N	1:A:61:PRO:CD	2.80	0.45
1:B:22:ALA:O	1:B:23:ILE:CB	2.60	0.45
1:H:179:ASP:OD1	1:H:179:ASP:C	2.58	0.45
1:D:17:HIS:HA	1:D:18:PRO:HA	1.54	0.45
1:G:59:ASP:HA	1:G:62:ARG:HD2	1.98	0.45
1:C:255:GLU:O	1:C:259[B]:ARG:HG3	2.17	0.45
1:D:60:THR:HB	1:D:61:PRO:HD3	1.98	0.45
1:F:4[B]:LYS:HE2	1:F:50:GLU:HG2	1.97	0.45
1:F:209:ARG:HD2	5:F:2802:HOH:O	2.17	0.45
1:G:23:ILE:HD13	1:G:23:ILE:HG21	1.65	0.45
1:H:273:ALA:N	1:H:274:PRO:HD2	2.32	0.45
1:D:265:ALA:HB1	1:D:288:LEU:HD22	1.99	0.45
1:D:281:GLY:O	1:D:285:LYS:HG3	2.17	0.45
1:E:130[A]:THR:O	1:E:130[A]:THR:HG23	2.16	0.45
1:C:60:THR:N	1:C:61:PRO:HD2	2.30	0.45
1:C:115:GLY:HA3	1:C:221:TYR:CD2	2.52	0.45
1:D:14:THR:O	1:D:17:HIS:CE1	2.69	0.45
1:G:60:THR:HB	1:G:61:PRO:HD3	1.99	0.44
1:C:18:PRO:HD3	1:D:280:TYR:CD1	2.52	0.44
1:D:65:GLN:CG	5:D:2631:HOH:O	2.54	0.44
1:D:119:HIS:HB3	5:D:2568:HOH:O	2.16	0.44
1:D:209:ARG:HG2	5:D:2787:HOH:O	2.16	0.44
1:B:23:ILE:HG13	1:B:24:SER:H	1.83	0.44
1:A:8:LEU:HD23	1:A:88:LEU:HD22	1.99	0.44
1:F:112:LEU:C	1:F:112:LEU:HD23	2.43	0.44
1:B:16:LEU:HD12	1:B:25:LYS:HB2	2.00	0.44
1:E:13:GLY:O	1:E:15:ARG:N	2.51	0.44
1:E:82:GLN:HG2	1:E:84:SER:O	2.17	0.44
1:E:112:LEU:HA	5:E:2623:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ARG:HD3	5:G:2820:HOH:O	2.16	0.44
1:D:62:ARG:HG2	5:D:2638:HOH:O	2.17	0.43
1:F:160:GLU:CD	5:F:2770:HOH:O	2.61	0.43
1:B:192:SER:O	1:B:195:GLY:N	2.43	0.43
1:E:155:LYS:HG2	5:E:2564:HOH:O	2.18	0.43
1:F:4[A]:LYS:NZ	1:F:102:ASP:OD2	2.39	0.43
1:F:249:LYS:HB3	1:F:252[B]:CYS:SG	2.59	0.43
1:A:161:GLU:O	1:A:194:ARG:NH2	2.52	0.43
1:C:29:PRO:HD3	1:D:28:LEU:HD22	2.00	0.43
1:F:64:GLN:NE2	5:F:2689:HOH:O	2.47	0.43
1:B:18:PRO:O	1:B:19:ALA:C	2.60	0.43
1:E:225:ASP:OD1	1:E:227:GLY:N	2.50	0.43
1:D:31:TYR:CD1	1:D:240:ALA:HB2	2.54	0.43
1:D:56:THR:HB	1:D:57:PRO:CD	2.49	0.43
1:D:60:THR:N	1:D:61:PRO:CD	2.80	0.43
1:E:183:VAL:HG23	5:E:2572:HOH:O	2.19	0.43
1:H:277:LYS:HD2	5:H:2696:HOH:O	2.18	0.43
1:A:199:ILE:HA	1:A:199:ILE:HD12	1.74	0.43
1:E:269:GLU:OE1	1:E:288:LEU:HD13	2.19	0.43
1:D:12:SER:C	1:D:14:THR:H	2.19	0.43
1:C:183:VAL:HG23	5:C:2580:HOH:O	2.18	0.43
1:C:260:GLN:NE2	1:C:262:TRP:CH2	2.87	0.43
1:F:86:ASP:C	1:F:196[B]:GLU:OE1	2.62	0.43
1:H:282:GLN:HG2	5:H:2776:HOH:O	2.19	0.43
1:A:237[B]:GLN:HG2	1:B:233:LEU:HD11	2.00	0.42
1:B:129:GLN:O	1:E:208:GLU:HG2	2.19	0.42
1:D:194:ARG:HD3	1:D:198:GLU:OE2	2.19	0.42
1:G:273:ALA:CB	1:G:274:PRO:CD	2.95	0.42
1:D:15:ARG:CB	5:D:2632:HOH:O	2.66	0.42
1:A:60:THR:HB	1:A:61:PRO:HD3	2.00	0.42
1:B:50:GLU:C	1:B:51:ILE:HG13	2.44	0.42
1:B:286:ARG:NH1	1:B:290:GLU:OE1	2.53	0.42
1:E:192:SER:CB	1:E:193:PRO:CD	2.97	0.42
1:E:184:ASP:O	1:E:187:ARG:HB2	2.20	0.42
1:H:85:PRO:HB2	5:H:2780:HOH:O	2.19	0.42
1:D:15:ARG:HB3	5:D:2632:HOH:O	2.20	0.42
1:D:64:GLN:HG2	1:D:79:TYR:CE1	2.54	0.42
1:E:187:ARG:CD	5:E:2717:HOH:O	2.64	0.42
1:D:16:LEU:O	1:D:19:ALA:HB3	2.19	0.42
1:D:249:LYS:HE3	5:D:2612:HOH:O	2.19	0.42
1:F:18:PRO:O	1:F:19:ALA:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114[B]:TYR:CD2	1:F:114[B]:TYR:C	2.94	0.42
1:D:41:SER:HB2	1:D:256:ILE:CD1	2.49	0.42
1:F:144:ARG:NH1	1:F:145:TYR:OH	2.53	0.42
1:H:41:SER:HB2	1:H:256:ILE:HD12	2.01	0.42
1:D:15:ARG:CG	5:D:2632:HOH:O	2.56	0.42
1:E:62:ARG:HH11	1:E:62:ARG:HD2	1.75	0.42
1:B:141:ASP:CB	5:B:2787:HOH:O	2.18	0.42
1:C:287:LEU:HD23	1:C:287:LEU:HA	1.71	0.42
1:B:23:ILE:HG12	1:B:27:LEU:CD1	2.43	0.41
1:B:192:SER:O	1:B:193:PRO:C	2.62	0.41
1:C:34:PRO:HD3	1:D:19:ALA:HA	2.01	0.41
1:C:55:SER:OG	1:C:56:THR:N	2.50	0.41
1:C:123:GLY:O	1:C:124:SER:C	2.62	0.41
1:C:252[A]:CYS:SG	1:C:284:LEU:HD21	2.60	0.41
1:F:271:LEU:O	1:F:274:PRO:HD2	2.20	0.41
1:G:15:ARG:NH1	5:G:2868:HOH:O	2.52	0.41
1:H:289:THR:HG23	5:H:2722:HOH:O	2.19	0.41
1:E:249:LYS:HB3	1:E:252[B]:CYS:SG	2.60	0.41
1:G:35[A]:MET:HE2	1:G:226:THR:OG1	2.19	0.41
1:A:15:ARG:HG3	1:A:15:ARG:NH1	2.27	0.41
1:D:145:TYR:HD2	2:D:2503:G1P:H5	1.86	0.41
1:H:199:ILE:HD12	1:H:199:ILE:HA	1.81	0.41
1:B:130:THR:HB	1:E:207:LEU:HG	2.02	0.41
1:D:26:GLN:HB2	1:D:63:PHE:HZ	1.85	0.41
1:G:16:LEU:O	1:G:229:HIS:HE1	2.04	0.41
1:F:16:LEU:HD21	1:F:228:THR:C	2.45	0.41
1:G:112:LEU:HD23	1:G:112:LEU:C	2.46	0.41
1:H:184:ASP:OD1	1:H:187:ARG:NH1	2.53	0.41
1:F:58:GLN:HB2	5:F:2711:HOH:O	2.20	0.41
1:G:199:ILE:HD12	1:G:199:ILE:HA	1.91	0.41
1:E:15:ARG:HG3	5:E:2691:HOH:O	2.20	0.41
1:C:155:LYS:HG2	5:C:2699:HOH:O	2.21	0.41
1:D:30:VAL:HB	1:D:38:TYR:CE1	2.56	0.41
1:E:35[B]:MET:SD	1:E:226:THR:HG21	2.61	0.41
1:E:119:HIS:HB3	5:E:2563:HOH:O	2.21	0.41
1:E:189:LEU:HD11	1:E:202:VAL:HG23	2.03	0.41
1:H:15:ARG:HG3	1:H:15:ARG:HH11	1.86	0.41
1:B:273:ALA:N	1:B:274:PRO:HD2	2.35	0.41
1:E:204:ARG:HH11	1:E:204:ARG:HD2	1.66	0.41
1:A:237[A]:GLN:HA	1:B:233:LEU:HD21	2.02	0.41
1:B:179:ASP:C	1:B:179:ASP:OD1	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:O	1:B:211:GLN:HG3	2.20	0.41
1:E:83:PRO:HD2	5:E:2625:HOH:O	2.20	0.41
1:E:251:ALA:O	1:E:253:PRO:HD3	2.21	0.41
1:F:287:LEU:HD23	1:F:287:LEU:HA	1.88	0.41
1:H:249:LYS:HB2	1:H:252[B]:CYS:SG	2.61	0.41
1:D:112:LEU:C	1:D:112:LEU:CD2	2.92	0.40
1:A:59:ASP:O	1:A:60:THR:C	2.62	0.40
1:A:273:ALA:N	1:A:274:PRO:CD	2.84	0.40
1:B:225:ASP:OD1	1:B:225:ASP:C	2.65	0.40
1:A:15:ARG:NH1	3:A:2507:SO4:O3	2.53	0.40
1:C:151:ASP:C	1:C:151:ASP:OD1	2.64	0.40
1:D:64:GLN:HG2	1:D:79:TYR:CD1	2.56	0.40
1:E:59:ASP:OD1	1:E:62:ARG:NH1	2.53	0.40
1:C:204:ARG:HH11	1:C:204:ARG:HD2	1.69	0.40
1:F:249:LYS:CB	1:F:252[B]:CYS:SG	3.10	0.40
1:G:16:LEU:HD23	1:G:16:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	296/293 (101%)	290 (98%)	6 (2%)	0	100	100
1	B	298/293 (102%)	293 (98%)	3 (1%)	2 (1%)	18	7
1	C	295/293 (101%)	287 (97%)	6 (2%)	2 (1%)	18	7
1	D	295/293 (101%)	284 (96%)	7 (2%)	4 (1%)	9	1
1	E	294/293 (100%)	279 (95%)	12 (4%)	3 (1%)	12	3
1	F	296/293 (101%)	289 (98%)	5 (2%)	2 (1%)	18	7
1	G	295/293 (101%)	291 (99%)	3 (1%)	1 (0%)	36	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	292/293 (100%)	285 (98%)	7 (2%)	0	100	100
All	All	2361/2344 (101%)	2298 (97%)	49 (2%)	14 (1%)	21	10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	THR
1	E	14	THR
1	B	23	ILE
1	F	31	TYR
1	B	31	TYR
1	C	31	TYR
1	D	16	LEU
1	D	31	TYR
1	E	31	TYR
1	F	14	THR
1	G	31	TYR
1	C	15	ARG
1	E	12	SER
1	D	17	HIS

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	245/240 (102%)	243 (99%)	2 (1%)	73	68
1	B	247/240 (103%)	242 (98%)	5 (2%)	48	33
1	C	244/240 (102%)	238 (98%)	6 (2%)	42	26
1	D	244/240 (102%)	240 (98%)	4 (2%)	55	43
1	E	243/240 (101%)	231 (95%)	12 (5%)	22	7
1	F	245/240 (102%)	240 (98%)	5 (2%)	48	33
1	G	244/240 (102%)	241 (99%)	3 (1%)	63	53
1	H	241/240 (100%)	235 (98%)	6 (2%)	42	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1953/1920 (102%)	1910 (98%)	43 (2%)	45 30

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	196	GLU
1	B	2	LYS
1	B	20	THR
1	B	28	LEU
1	B	194	ARG
1	B	278	ASN
1	C	12	SER
1	C	14	THR
1	C	24	SER
1	C	26	GLN
1	C	81	VAL
1	C	164	LEU
1	D	12	SER
1	D	24	SER
1	D	119	HIS
1	D	164	LEU
1	E	15	ARG
1	E	23	ILE
1	E	27	LEU
1	E	36	ILE
1	E	90	GLN
1	E	119	HIS
1	E	164	LEU
1	E	165	GLU
1	E	168	SER
1	E	194	ARG
1	E	225	ASP
1	E	270	LYS
1	F	1	MET
1	F	24	SER
1	F	148	VAL
1	F	197	LEU
1	F	199	ILE
1	G	2	LYS
1	G	62	ARG
1	G	278	ASN

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Mol	Chain	Res	Type
1	H	2	LYS
1	H	15	ARG
1	H	111	ASN
1	H	112	LEU
1	H	225	ASP
1	H	278	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	65	GLN
1	A	72	ASN
1	A	282	GLN
1	C	26	GLN
1	C	64	GLN
1	C	65	GLN
1	C	119	HIS
1	C	181	GLN
1	C	211	GLN
1	C	229	HIS
1	C	260	GLN
1	D	26	GLN
1	D	181	GLN
1	D	211	GLN
1	D	229	HIS
1	E	26	GLN
1	E	246	GLN
1	F	65	GLN
1	F	181	GLN
1	F	211	GLN
1	F	244	ASN
1	G	26	GLN
1	G	229	HIS
1	G	246	GLN
1	H	26	GLN
1	H	180	GLN
1	H	278	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SO4	B	2511	-	4,4,4	0.68	0	6,6,6	1.04	0
4	THM	D	2541	-	18,18,18	1.97	5 (27%)	26,26,26	3.27	11 (42%)
4	THM	G	2544	-	18,18,18	2.37	5 (27%)	26,26,26	2.42	11 (42%)
3	SO4	C	2513	-	4,4,4	1.01	0	6,6,6	0.58	0
4	THM	H	2545	-	18,18,18	2.63	10 (55%)	26,26,26	3.33	10 (38%)
3	SO4	D	2512	-	4,4,4	0.67	0	6,6,6	0.66	0
3	SO4	G	2525	-	4,4,4	0.59	0	6,6,6	1.12	0
4	THM	C	2540	-	18,18,18	2.46	8 (44%)	26,26,26	2.41	11 (42%)
2	G1P	C	2502	-	15,16,16	2.09	6 (40%)	24,24,24	3.90	8 (33%)
3	SO4	D	2517	-	4,4,4	0.19	0	6,6,6	0.70	0
2	G1P	B	2501	-	15,16,16	2.24	4 (26%)	24,24,24	4.67	8 (33%)
3	SO4	H	2529	-	4,4,4	0.35	0	6,6,6	1.02	0
4	THM	H	2537	-	18,18,18	3.17	9 (50%)	26,26,26	2.74	10 (38%)
3	SO4	D	2514	-	4,4,4	0.25	0	6,6,6	1.23	1 (16%)
4	THM	D	2533	-	18,18,18	2.49	5 (27%)	26,26,26	2.62	11 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G1P	A	2500	-	15,16,16	1.99	5 (33%)	24,24,24	2.63	7 (29%)
2	G1P	E	2504	-	15,16,16	2.01	4 (26%)	24,24,24	5.12	9 (37%)
3	SO4	C	2515	-	4,4,4	0.44	0	6,6,6	0.61	0
3	SO4	E	2527	-	4,4,4	0.90	0	6,6,6	0.69	0
4	THM	A	2530	-	18,18,18	2.60	8 (44%)	26,26,26	3.46	15 (57%)
4	THM	F	2543	-	18,18,18	2.26	5 (27%)	26,26,26	2.79	8 (30%)
4	THM	B	2539	-	18,18,18	2.64	5 (27%)	26,26,26	2.75	11 (42%)
4	THM	B	2531	-	18,18,18	2.59	7 (38%)	26,26,26	2.90	14 (53%)
4	THM	A	2538	-	18,18,18	2.89	10 (55%)	26,26,26	2.64	10 (38%)
3	SO4	E	2520	-	4,4,4	0.31	0	6,6,6	0.34	0
4	THM	E	2542	-	18,18,18	2.85	10 (55%)	26,26,26	2.37	10 (38%)
3	SO4	D	2516	-	4,4,4	0.70	0	6,6,6	0.16	0
3	SO4	H	2518	-	4,4,4	0.47	0	6,6,6	0.39	0
4	THM	E	2534	-	18,18,18	2.49	6 (33%)	26,26,26	3.65	14 (53%)
3	SO4	A	2507	-	4,4,4	0.94	0	6,6,6	0.95	1 (16%)
2	G1P	G	2505	-	15,16,16	1.68	3 (20%)	24,24,24	3.41	8 (33%)
2	G1P	H	2506	-	15,16,16	1.91	4 (26%)	24,24,24	3.82	5 (20%)
3	SO4	F	2519	-	4,4,4	0.44	0	6,6,6	0.63	0
3	SO4	G	2523	-	4,4,4	0.54	0	6,6,6	0.87	0
3	SO4	H	2526	-	4,4,4	0.41	0	6,6,6	0.42	0
2	G1P	D	2503	-	15,16,16	2.01	4 (26%)	24,24,24	3.64	10 (41%)
3	SO4	F	2521	-	4,4,4	0.64	0	6,6,6	0.83	0
4	THM	F	2535	-	18,18,18	2.63	8 (44%)	26,26,26	3.64	19 (73%)
3	SO4	A	2508	-	4,4,4	0.75	0	6,6,6	0.94	0
3	SO4	B	2528	-	4,4,4	0.69	0	6,6,6	0.82	0
3	SO4	B	2510	-	4,4,4	0.18	0	6,6,6	0.52	0
3	SO4	C	2509	-	4,4,4	0.61	0	6,6,6	1.05	1 (16%)
3	SO4	F	2522	-	4,4,4	0.33	0	6,6,6	0.54	0
4	THM	C	2532	-	18,18,18	2.50	8 (44%)	26,26,26	3.11	16 (61%)
3	SO4	F	2524	-	4,4,4	0.39	0	6,6,6	0.81	0
4	THM	G	2536	-	18,18,18	2.47	9 (50%)	26,26,26	3.09	14 (53%)

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
4	THM	D	2541	-	-	0/6/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	THM	G	2544	-	-	0/6/18/18	0/2/2/2
4	THM	H	2545	-	-	0/6/18/18	0/2/2/2
2	G1P	C	2502	-	-	1/7/27/27	0/1/1/1
2	G1P	B	2501	-	-	0/7/27/27	0/1/1/1
4	THM	H	2537	-	-	1/6/18/18	0/2/2/2
4	THM	D	2533	-	-	1/6/18/18	0/2/2/2
2	G1P	A	2500	-	-	0/7/27/27	0/1/1/1
4	THM	F	2543	-	-	0/6/18/18	0/2/2/2
2	G1P	E	2504	-	-	0/7/27/27	0/1/1/1
4	THM	A	2530	-	-	0/6/18/18	0/2/2/2
4	THM	B	2539	-	-	0/6/18/18	0/2/2/2
4	THM	B	2531	-	-	0/6/18/18	0/2/2/2
4	THM	A	2538	-	-	0/6/18/18	0/2/2/2
4	THM	E	2542	-	-	0/6/18/18	0/2/2/2
4	THM	E	2534	-	-	2/6/18/18	0/2/2/2
2	G1P	G	2505	-	-	0/7/27/27	0/1/1/1
2	G1P	H	2506	-	-	1/7/27/27	0/1/1/1
4	THM	C	2532	-	-	0/6/18/18	0/2/2/2
2	G1P	D	2503	-	-	0/7/27/27	0/1/1/1
4	THM	F	2535	-	-	0/6/18/18	0/2/2/2
4	THM	C	2540	-	-	0/6/18/18	0/2/2/2
4	THM	G	2536	-	-	0/6/18/18	0/2/2/2

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2539	THM	O2-C2	7.45	1.36	1.23
4	B	2531	THM	O2-C2	6.72	1.35	1.23
4	G	2544	THM	O2-C2	6.09	1.33	1.23
4	D	2533	THM	O4-C4	6.08	1.35	1.23
4	H	2537	THM	C4-C5	-5.78	1.35	1.44
4	A	2538	THM	O2-C2	5.73	1.33	1.23
4	H	2537	THM	O4-C4	5.44	1.33	1.23
4	F	2535	THM	O4-C4	5.38	1.33	1.23
4	C	2532	THM	O4-C4	5.32	1.33	1.23
4	C	2540	THM	O4-C4	5.29	1.33	1.23
4	H	2537	THM	C2-N1	-5.27	1.30	1.38
4	F	2535	THM	O3'-C3'	5.24	1.54	1.43
4	H	2545	THM	O2-C2	5.13	1.32	1.23
4	H	2537	THM	O2-C2	5.02	1.31	1.23
4	A	2538	THM	C2-N1	-4.98	1.30	1.38
4	C	2532	THM	C2-N1	-4.98	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2542	THM	O4-C4	4.88	1.32	1.23
4	E	2534	THM	O2-C2	4.88	1.31	1.23
4	D	2541	THM	O2-C2	4.85	1.31	1.23
2	B	2501	G1P	P-O1P	4.84	1.65	1.50
4	F	2543	THM	O2-C2	4.84	1.31	1.23
4	E	2542	THM	C4-N3	-4.83	1.29	1.38
4	E	2534	THM	O4-C4	4.78	1.32	1.23
4	H	2545	THM	C4-C5	-4.75	1.37	1.44
4	G	2536	THM	C2-N3	-4.71	1.29	1.38
4	B	2531	THM	O4-C4	4.71	1.32	1.23
4	C	2540	THM	C2-N1	-4.61	1.31	1.38
2	E	2504	G1P	P-O3P	4.56	1.71	1.54
4	F	2543	THM	C2-N1	-4.54	1.31	1.38
2	A	2500	G1P	P-O2P	4.47	1.71	1.54
4	E	2534	THM	C2-N1	-4.45	1.31	1.38
4	A	2538	THM	O4-C4	4.43	1.32	1.23
4	B	2539	THM	C4-N3	-4.43	1.30	1.38
4	E	2542	THM	O2-C2	4.43	1.30	1.23
4	G	2536	THM	C6-N1	-4.39	1.30	1.38
4	D	2533	THM	C2-N1	-4.37	1.31	1.38
4	D	2533	THM	O2-C2	4.35	1.30	1.23
4	F	2543	THM	C4-N3	-4.35	1.30	1.38
2	B	2501	G1P	P-O2P	4.34	1.70	1.54
4	E	2542	THM	C2-N3	-4.33	1.30	1.38
4	A	2530	THM	C6-N1	-4.32	1.30	1.38
2	D	2503	G1P	P-O2P	4.29	1.70	1.54
2	D	2503	G1P	P-O3P	4.27	1.70	1.54
4	A	2530	THM	C4-N3	-4.21	1.31	1.38
4	A	2530	THM	O4-C4	4.21	1.31	1.23
2	C	2502	G1P	P-O2P	4.15	1.70	1.54
2	E	2504	G1P	P-O2P	4.08	1.70	1.54
2	H	2506	G1P	P-O1P	4.03	1.63	1.50
4	F	2535	THM	C6-N1	-4.01	1.31	1.38
4	E	2542	THM	C4-C5	-4.00	1.38	1.44
4	A	2538	THM	O4'-C4'	-3.97	1.36	1.45
2	G	2505	G1P	P-O2P	3.96	1.69	1.54
4	B	2531	THM	C6-C5	3.95	1.41	1.34
4	A	2530	THM	O3'-C3'	3.95	1.51	1.43
4	E	2534	THM	C4-C5	-3.91	1.38	1.44
4	H	2545	THM	C1'-N1	-3.89	1.38	1.48
4	A	2538	THM	C4-C5	-3.88	1.38	1.44
4	H	2537	THM	C4-N3	-3.87	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2537	THM	C6-N1	-3.85	1.31	1.38
4	G	2544	THM	C4-N3	-3.84	1.31	1.38
2	H	2506	G1P	P-O2P	3.83	1.69	1.54
4	B	2539	THM	C4-C5	-3.79	1.38	1.44
4	C	2532	THM	C4-N3	-3.79	1.31	1.38
4	C	2540	THM	C4-C5	-3.68	1.38	1.44
2	B	2501	G1P	P-O3P	3.67	1.68	1.54
4	G	2536	THM	O2-C2	3.67	1.29	1.23
4	E	2542	THM	C2-N1	-3.67	1.32	1.38
4	F	2535	THM	O2-C2	3.67	1.29	1.23
4	F	2535	THM	C2-N3	-3.67	1.31	1.38
2	C	2502	G1P	P-O3P	3.61	1.68	1.54
4	G	2544	THM	C4-C5	-3.56	1.39	1.44
4	F	2543	THM	C4-C5	-3.51	1.39	1.44
4	B	2531	THM	O3'-C3'	3.46	1.50	1.43
4	A	2530	THM	C4-C5	-3.43	1.39	1.44
4	E	2534	THM	C2-N3	-3.42	1.32	1.38
4	A	2530	THM	C2-N1	-3.41	1.33	1.38
2	A	2500	G1P	P-O3P	3.40	1.67	1.54
4	A	2538	THM	C4-N3	-3.39	1.32	1.38
4	H	2537	THM	C2-N3	-3.38	1.32	1.38
4	D	2541	THM	C6-C5	3.34	1.40	1.34
2	H	2506	G1P	P-O3P	3.32	1.67	1.54
4	H	2545	THM	C2-N3	-3.25	1.32	1.38
4	C	2540	THM	C2'-C1'	-3.24	1.43	1.52
4	G	2536	THM	O4-C4	3.23	1.29	1.23
4	H	2545	THM	C4-N3	-3.21	1.32	1.38
4	G	2544	THM	C6-N1	-3.19	1.32	1.38
4	D	2541	THM	C4-N3	-3.17	1.32	1.38
4	D	2541	THM	C2-N1	-3.11	1.33	1.38
4	D	2533	THM	C4-C5	-3.09	1.39	1.44
2	A	2500	G1P	P-O1	3.05	1.64	1.59
4	A	2530	THM	C2-N3	-3.04	1.32	1.38
2	B	2501	G1P	O3-C3	2.99	1.50	1.43
2	E	2504	G1P	P-O1P	2.98	1.59	1.50
4	B	2539	THM	C2-N1	-2.96	1.33	1.38
4	G	2536	THM	C4-N3	-2.95	1.33	1.38
2	D	2503	G1P	P-O1P	2.89	1.59	1.50
4	C	2532	THM	C6-N1	-2.87	1.33	1.38
4	C	2532	THM	O3'-C3'	2.82	1.49	1.43
2	G	2505	G1P	P-O3P	2.78	1.65	1.54
2	C	2502	G1P	O2-C2	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2502	G1P	P-O1P	2.69	1.58	1.50
4	A	2530	THM	C6-C5	2.67	1.39	1.34
4	C	2532	THM	C4-C5	-2.67	1.40	1.44
2	H	2506	G1P	P-O1	2.64	1.64	1.59
4	H	2545	THM	C6-N1	-2.63	1.33	1.38
4	C	2540	THM	C2-N3	-2.63	1.33	1.38
4	D	2533	THM	C4-N3	-2.61	1.34	1.38
4	F	2535	THM	C6-C5	2.53	1.38	1.34
4	C	2540	THM	O2-C2	2.53	1.27	1.23
4	B	2539	THM	O4-C4	2.52	1.28	1.23
4	G	2536	THM	O3'-C3'	2.51	1.48	1.43
4	E	2542	THM	C1'-N1	-2.49	1.41	1.48
4	H	2545	THM	O4'-C4'	-2.49	1.39	1.45
4	D	2541	THM	C4-C5	-2.49	1.40	1.44
4	H	2545	THM	C2-N1	-2.48	1.34	1.38
4	G	2536	THM	C6-C5	2.47	1.38	1.34
4	E	2542	THM	C6-C5	2.46	1.38	1.34
4	B	2531	THM	C2-N3	-2.42	1.33	1.38
4	G	2536	THM	C2-N1	-2.40	1.34	1.38
2	A	2500	G1P	P-O1P	2.38	1.57	1.50
4	E	2542	THM	C6-N1	-2.37	1.34	1.38
4	G	2544	THM	C2-N1	-2.36	1.34	1.38
4	H	2537	THM	O3'-C3'	2.36	1.48	1.43
4	C	2540	THM	C5'-C4'	2.35	1.59	1.51
4	C	2532	THM	C2-N3	-2.33	1.33	1.38
4	B	2531	THM	C2-N1	-2.32	1.34	1.38
4	F	2535	THM	C1'-N1	-2.31	1.42	1.48
4	H	2545	THM	O4-C4	2.31	1.27	1.23
4	A	2538	THM	C6-C5	2.28	1.38	1.34
2	G	2505	G1P	P-O1	2.27	1.63	1.59
2	C	2502	G1P	O3-C3	2.23	1.48	1.43
4	A	2538	THM	C6-N1	-2.23	1.34	1.38
4	F	2535	THM	C4-C5	-2.20	1.41	1.44
4	F	2543	THM	O5'-C5'	-2.17	1.33	1.42
4	C	2540	THM	O4'-C4'	-2.16	1.40	1.45
4	E	2542	THM	O4'-C4'	-2.12	1.40	1.45
2	D	2503	G1P	C4-C5	2.10	1.57	1.53
4	E	2534	THM	C6-N1	-2.09	1.34	1.38
4	A	2538	THM	C2'-C1'	-2.07	1.46	1.52
4	A	2538	THM	O4'-C1'	-2.07	1.37	1.42
4	B	2531	THM	C4-N3	-2.06	1.35	1.38
4	H	2537	THM	C2'-C1'	-2.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2502	G1P	C4-C5	2.03	1.57	1.53
4	G	2536	THM	O4'-C4'	-2.03	1.40	1.45
4	H	2545	THM	C5'-C4'	2.03	1.58	1.51
2	E	2504	G1P	P-O1	2.03	1.63	1.59
4	C	2532	THM	O2-C2	2.03	1.26	1.23
2	A	2500	G1P	O5-C5	-2.01	1.39	1.44

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2504	G1P	O5-C1-O1	-22.82	81.54	111.36
2	B	2501	G1P	O5-C1-O1	-18.25	87.50	111.36
2	H	2506	G1P	O5-C1-O1	-15.76	90.76	111.36
2	C	2502	G1P	O5-C1-O1	-15.28	91.39	111.36
2	D	2503	G1P	O5-C1-O1	-14.59	92.29	111.36
2	G	2505	G1P	O5-C1-O1	-13.71	93.44	111.36
2	A	2500	G1P	O5-C1-O1	-8.66	100.04	111.36
4	E	2534	THM	O4-C4-C5	-8.47	115.23	124.92
2	C	2502	G1P	O5-C1-C2	8.36	127.54	110.37
4	D	2541	THM	C5-C4-N3	8.06	122.33	115.32
4	H	2545	THM	C5-C4-N3	7.90	122.19	115.32
4	H	2545	THM	O4-C4-C5	-7.69	116.12	124.92
4	F	2543	THM	C5-C4-N3	7.40	121.75	115.32
2	B	2501	G1P	O5-C1-C2	7.19	125.13	110.37
4	E	2534	THM	C5-C4-N3	7.16	121.55	115.32
4	B	2539	THM	O4-C4-C5	-6.80	117.14	124.92
4	H	2537	THM	O4'-C4'-C5'	6.73	123.45	109.22
4	A	2530	THM	C4-N3-C2	-6.71	118.55	127.34
4	H	2545	THM	C4-N3-C2	-6.53	118.77	127.34
4	A	2530	THM	N3-C2-N1	6.53	123.39	114.89
2	H	2506	G1P	O5-C1-C2	6.46	123.64	110.37
4	G	2536	THM	C5M-C5-C4	6.43	125.64	118.78
4	D	2541	THM	O4'-C4'-C5'	6.38	122.71	109.22
4	C	2540	THM	O4'-C4'-C5'	6.35	122.64	109.22
4	D	2541	THM	C5-C6-N1	-6.32	116.45	123.31
4	A	2538	THM	C5-C4-N3	6.32	120.82	115.32
4	F	2543	THM	O4'-C4'-C5'	6.28	122.49	109.22
4	D	2541	THM	C4-N3-C2	-6.20	119.22	127.34
2	E	2504	G1P	O5-C1-C2	6.03	122.76	110.37
4	F	2543	THM	C4-N3-C2	-5.96	119.53	127.34
4	A	2538	THM	O4-C4-C5	-5.92	118.15	124.92
4	B	2539	THM	C5-C6-N1	-5.89	116.91	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2534	THM	C4-N3-C2	-5.83	119.69	127.34
4	C	2532	THM	N3-C2-N1	5.82	122.47	114.89
4	H	2545	THM	C5-C6-N1	-5.79	117.03	123.31
2	B	2501	G1P	O4-C4-C3	-5.77	96.78	110.38
4	E	2542	THM	C5-C6-N1	-5.69	117.13	123.31
4	A	2530	THM	C5-C6-N1	-5.68	117.14	123.31
4	F	2535	THM	O2-C2-N1	-5.66	115.43	122.80
4	F	2535	THM	C2'-C3'-C4'	-5.65	91.34	102.80
4	F	2535	THM	C4-N3-C2	-5.60	120.00	127.34
4	C	2532	THM	C5'-C4'-C3'	5.58	128.73	114.82
4	B	2531	THM	O4-C4-C5	-5.56	118.56	124.92
4	F	2535	THM	C5'-C4'-C3'	5.55	128.66	114.82
4	E	2542	THM	O4'-C4'-C5'	5.47	120.78	109.22
4	H	2545	THM	O4'-C4'-C5'	5.43	120.71	109.22
4	E	2534	THM	O4'-C4'-C5'	5.42	120.69	109.22
4	F	2535	THM	O4-C4-C5	-5.41	118.73	124.92
4	G	2536	THM	C5'-C4'-C3'	5.38	128.24	114.82
4	C	2532	THM	C4-N3-C2	-5.35	120.33	127.34
4	A	2530	THM	O4'-C4'-C5'	5.34	120.51	109.22
2	D	2503	G1P	O5-C1-C2	5.32	121.30	110.37
4	E	2534	THM	C5'-C4'-C3'	5.32	128.07	114.82
4	G	2536	THM	C5-C6-N1	-5.31	117.54	123.31
4	A	2530	THM	C5'-C4'-C3'	5.21	127.82	114.82
4	B	2531	THM	O4'-C1'-N1	-5.19	98.65	107.86
2	G	2505	G1P	O5-C1-C2	5.19	121.04	110.37
4	B	2539	THM	O4'-C4'-C5'	5.19	120.18	109.22
4	C	2532	THM	O4'-C4'-C5'	5.14	120.09	109.22
4	B	2539	THM	C5-C4-N3	5.11	119.77	115.32
4	H	2537	THM	C5-C4-N3	5.07	119.73	115.32
4	A	2538	THM	C4-N3-C2	-5.03	120.74	127.34
4	F	2535	THM	C5-C6-N1	-5.02	117.86	123.31
4	D	2533	THM	O4-C4-C5	-4.96	119.24	124.92
4	E	2534	THM	C5-C6-N1	-4.94	117.95	123.31
2	B	2501	G1P	O1-C1-C2	-4.86	99.48	108.38
4	A	2530	THM	C5-C4-N3	4.86	119.54	115.32
4	H	2537	THM	C5'-C4'-C3'	4.83	126.86	114.82
4	E	2534	THM	C2'-C3'-C4'	-4.82	93.02	102.80
2	A	2500	G1P	O5-C1-C2	4.79	120.22	110.37
2	H	2506	G1P	C4-C3-C2	-4.77	102.45	110.83
2	B	2501	G1P	O4-C4-C5	4.76	121.06	109.32
4	G	2536	THM	C5M-C5-C6	-4.75	116.43	122.85
4	G	2544	THM	O4-C4-C5	-4.72	119.52	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2530	THM	O2-C2-N1	-4.69	116.70	122.80
4	C	2532	THM	C5-C6-N1	-4.65	118.26	123.31
4	G	2536	THM	O4-C4-C5	-4.64	119.61	124.92
4	A	2530	THM	C2'-C3'-C4'	-4.63	93.40	102.80
4	F	2535	THM	O4'-C4'-C3'	-4.62	95.12	105.65
2	A	2500	G1P	O4-C4-C3	-4.61	99.52	110.38
4	H	2537	THM	C4-N3-C2	-4.60	121.31	127.34
4	G	2544	THM	C4-N3-C2	-4.53	121.40	127.34
4	D	2533	THM	C5-C6-N1	-4.52	118.40	123.31
4	D	2533	THM	C5'-C4'-C3'	4.50	126.03	114.82
4	F	2535	THM	N3-C2-N1	4.48	120.72	114.89
4	B	2531	THM	O4'-C4'-C5'	4.38	118.48	109.22
4	D	2533	THM	O4'-C4'-C5'	4.34	118.38	109.22
4	D	2541	THM	O4-C4-C5	-4.31	119.99	124.92
4	G	2536	THM	C4-N3-C2	-4.31	121.69	127.34
4	D	2533	THM	C4-N3-C2	-4.29	121.72	127.34
4	F	2543	THM	C5-C6-N1	-4.26	118.69	123.31
4	G	2536	THM	C5-C4-N3	4.23	119.00	115.32
4	D	2533	THM	C5-C4-N3	4.21	118.98	115.32
4	B	2531	THM	C5-C4-N3	4.14	118.92	115.32
4	G	2544	THM	C5M-C5-C6	-4.09	117.31	122.85
4	C	2532	THM	O2-C2-N1	-4.08	117.49	122.80
4	D	2541	THM	O2-C2-N1	-4.05	117.52	122.80
4	E	2542	THM	N3-C2-N1	4.05	120.17	114.89
4	H	2537	THM	N3-C2-N1	4.05	120.16	114.89
4	H	2545	THM	N3-C2-N1	4.04	120.15	114.89
2	B	2501	G1P	P-O1-C1	-4.03	112.73	123.54
4	B	2531	THM	C2'-C1'-N1	4.02	123.85	113.81
2	D	2503	G1P	C1-O5-C5	3.99	121.52	113.72
4	C	2540	THM	C4-N3-C2	-3.94	122.18	127.34
4	C	2532	THM	O3'-C3'-C2'	3.93	124.52	110.88
4	E	2534	THM	O4'-C4'-C3'	-3.92	96.71	105.65
4	B	2531	THM	C5-C6-N1	-3.91	119.07	123.31
4	B	2531	THM	O3'-C3'-C2'	3.90	124.41	110.88
4	G	2544	THM	C5M-C5-C4	3.84	122.88	118.78
4	G	2544	THM	C5-C4-N3	3.83	118.66	115.32
2	D	2503	G1P	O4-C4-C3	-3.82	101.37	110.38
4	F	2543	THM	N3-C2-N1	3.82	119.86	114.89
2	G	2505	G1P	P-O1-C1	-3.81	113.33	123.54
4	C	2540	THM	N3-C2-N1	3.80	119.84	114.89
4	B	2539	THM	C4-N3-C2	-3.78	122.38	127.34
4	A	2538	THM	O4'-C4'-C5'	3.75	117.15	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2534	THM	O2-C2-N1	-3.75	117.91	122.80
4	F	2535	THM	C5-C4-N3	3.74	118.57	115.32
4	A	2538	THM	C5-C6-N1	-3.73	119.26	123.31
4	F	2535	THM	O3'-C3'-C2'	3.68	123.66	110.88
4	F	2535	THM	C3'-C2'-C1'	-3.66	93.64	102.60
4	C	2540	THM	O3'-C3'-C2'	3.65	123.55	110.88
4	B	2531	THM	N3-C2-N1	3.64	119.63	114.89
2	B	2501	G1P	O5-C5-C4	3.63	116.25	109.70
4	F	2535	THM	O4'-C4'-C5'	3.61	116.85	109.22
4	F	2535	THM	C1'-N1-C2	-3.56	110.69	117.66
4	D	2541	THM	C6-N1-C2	3.56	124.85	121.30
4	B	2531	THM	C4-N3-C2	-3.54	122.70	127.34
4	E	2534	THM	C6-N1-C2	3.47	124.76	121.30
4	A	2530	THM	O4-C4-C5	-3.46	120.96	124.92
2	B	2501	G1P	C4-C3-C2	-3.46	104.76	110.83
4	C	2532	THM	O4'-C1'-N1	-3.45	101.75	107.86
2	D	2503	G1P	O4-C4-C5	3.44	117.79	109.32
4	D	2533	THM	N3-C2-N1	3.43	119.36	114.89
4	G	2536	THM	O4'-C4'-C5'	3.42	116.44	109.22
2	E	2504	G1P	C1-O5-C5	3.41	120.39	113.72
4	C	2540	THM	O2-C2-N1	-3.40	118.37	122.80
4	G	2536	THM	N3-C2-N1	3.40	119.32	114.89
2	A	2500	G1P	O5-C5-C4	3.36	115.76	109.70
4	H	2537	THM	C5-C6-N1	-3.34	119.69	123.31
4	G	2544	THM	O4'-C4'-C5'	3.30	116.19	109.22
4	C	2540	THM	C5M-C5-C4	3.30	122.30	118.78
2	E	2504	G1P	O5-C5-C4	3.29	115.63	109.70
4	H	2537	THM	C2'-C3'-C4'	-3.28	96.15	102.80
4	D	2533	THM	O4'-C1'-N1	-3.21	102.16	107.86
4	F	2543	THM	O3'-C3'-C2'	3.21	122.02	110.88
4	A	2538	THM	C4'-O4'-C1'	3.19	117.09	109.51
4	B	2531	THM	C5'-C4'-C3'	3.17	122.71	114.82
4	E	2542	THM	C5-C4-N3	3.14	118.05	115.32
4	G	2536	THM	C6-N1-C2	3.14	124.43	121.30
4	E	2534	THM	N3-C2-N1	3.12	118.95	114.89
2	C	2502	G1P	O4-C4-C3	-3.12	103.03	110.38
4	C	2532	THM	C2'-C3'-C4'	-3.10	96.51	102.80
4	E	2542	THM	C4-N3-C2	-3.07	123.31	127.34
4	E	2534	THM	O3'-C3'-C2'	3.07	121.54	110.88
4	C	2532	THM	C5-C4-N3	3.07	117.99	115.32
4	F	2535	THM	C1'-N1-C6	3.05	125.86	120.74
4	C	2540	THM	C5M-C5-C6	-3.03	118.75	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2544	THM	O3'-C3'-C2'	3.02	121.37	110.88
4	G	2544	THM	N3-C2-N1	3.01	118.81	114.89
4	D	2541	THM	N3-C2-N1	2.98	118.77	114.89
4	G	2544	THM	O2-C2-N1	-2.98	118.92	122.80
4	A	2530	THM	O3'-C3'-C2'	2.95	121.13	110.88
2	H	2506	G1P	O5-C5-C4	2.92	114.95	109.70
4	C	2532	THM	O4-C4-C5	-2.89	121.61	124.92
4	F	2535	THM	C2'-C1'-N1	2.89	121.03	113.81
2	H	2506	G1P	O4-C4-C3	-2.88	103.60	110.38
4	A	2538	THM	O3'-C3'-C2'	2.87	120.87	110.88
4	B	2531	THM	C2'-C3'-C4'	-2.87	96.98	102.80
4	B	2531	THM	O2-C2-N1	-2.86	119.07	122.80
4	A	2538	THM	N3-C2-N1	2.86	118.62	114.89
4	G	2544	THM	C5-C6-N1	-2.86	120.21	123.31
4	H	2545	THM	O4'-C4'-C3'	-2.84	99.18	105.65
4	H	2537	THM	C5M-C5-C4	2.81	121.79	118.78
2	C	2502	G1P	O4-C4-C5	2.81	116.25	109.32
2	C	2502	G1P	P-O1-C1	-2.77	116.09	123.54
4	A	2530	THM	O4'-C4'-C3'	-2.71	99.46	105.65
4	B	2539	THM	O2-C2-N1	-2.69	119.29	122.80
4	H	2545	THM	O2-C2-N1	-2.69	119.30	122.80
4	D	2541	THM	O5'-C5'-C4'	2.67	120.43	111.33
4	F	2535	THM	C5M-C5-C6	-2.67	119.24	122.85
4	H	2545	THM	O3'-C3'-C2'	2.66	120.11	110.88
4	H	2537	THM	O4'-C4'-C3'	-2.65	99.61	105.65
4	A	2530	THM	C5M-C5-C6	-2.64	119.28	122.85
4	E	2542	THM	O3'-C3'-C2'	2.62	119.98	110.88
3	D	2514	SO4	O4-S-O2	-2.62	95.87	109.56
2	C	2502	G1P	O2-C2-C1	2.61	116.29	110.08
4	G	2536	THM	O2-C2-N1	-2.61	119.40	122.80
2	E	2504	G1P	O4-C4-C3	-2.60	104.25	110.38
4	G	2536	THM	O3'-C3'-C2'	2.60	119.90	110.88
4	C	2540	THM	C5-C6-N1	-2.59	120.50	123.31
4	D	2533	THM	O3'-C3'-C2'	2.59	119.88	110.88
4	A	2530	THM	O4'-C1'-C2'	-2.58	101.43	106.25
4	C	2532	THM	O4'-C4'-C3'	-2.56	99.81	105.65
2	A	2500	G1P	C4-C3-C2	-2.55	106.35	110.83
4	F	2535	THM	O3'-C3'-C4'	2.55	119.75	110.07
4	A	2530	THM	C6-C5-C4	2.55	120.12	118.02
2	G	2505	G1P	O2P-P-O1P	-2.55	100.90	110.83
2	E	2504	G1P	O4-C4-C5	2.52	115.52	109.32
4	B	2539	THM	O3'-C3'-C2'	2.51	119.61	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2542	THM	C2'-C1'-N1	-2.51	107.55	113.81
4	A	2538	THM	O4'-C4'-C3'	-2.50	99.95	105.65
4	E	2542	THM	C5M-C5-C6	-2.50	119.47	122.85
4	A	2530	THM	O4'-C1'-N1	-2.48	103.47	107.86
2	E	2504	G1P	O3P-P-O1	2.45	115.39	105.85
2	A	2500	G1P	C1-O5-C5	2.44	118.48	113.72
4	B	2531	THM	C5M-C5-C4	2.43	121.38	118.78
4	D	2541	THM	C5'-C4'-C3'	-2.43	108.77	114.82
4	F	2535	THM	O4'-C1'-N1	-2.40	103.61	107.86
4	D	2541	THM	O3'-C3'-C2'	2.39	119.19	110.88
2	D	2503	G1P	O5-C5-C4	2.38	113.99	109.70
4	D	2533	THM	O2-C2-N1	-2.38	119.70	122.80
4	C	2532	THM	C6-C5-C4	2.37	119.98	118.02
4	H	2537	THM	O3'-C3'-C2'	2.36	119.07	110.88
4	G	2536	THM	O4'-C4'-C3'	-2.34	100.32	105.65
2	A	2500	G1P	O4-C4-C5	2.33	115.07	109.32
4	C	2532	THM	C5M-C5-C6	-2.32	119.71	122.85
2	G	2505	G1P	C4-C3-C2	-2.30	106.78	110.83
2	E	2504	G1P	O2-C2-C1	2.30	115.56	110.08
4	E	2534	THM	C1'-N1-C2	-2.28	113.20	117.66
4	G	2536	THM	C2'-C1'-N1	2.27	119.50	113.81
4	F	2543	THM	O4-C4-N3	-2.27	115.84	120.11
2	C	2502	G1P	C3-C4-C5	2.27	114.35	110.23
4	E	2542	THM	O2-C2-N1	-2.26	119.85	122.80
4	D	2533	THM	O4'-C4'-C3'	-2.26	100.49	105.65
4	B	2539	THM	C3'-C2'-C1'	-2.26	97.07	102.60
4	B	2531	THM	O5'-C5'-C4'	-2.25	103.68	111.33
4	H	2545	THM	C4'-O4'-C1'	2.24	114.84	109.51
4	C	2532	THM	C3'-C2'-C1'	-2.23	97.13	102.60
4	C	2540	THM	O4'-C1'-N1	-2.22	103.92	107.86
4	F	2543	THM	O4-C4-C5	-2.22	122.38	124.92
2	G	2505	G1P	C6-C5-C4	2.20	118.42	113.02
4	F	2535	THM	C5M-C5-C4	2.19	121.12	118.78
2	D	2503	G1P	O1-C1-C2	-2.19	104.37	108.38
2	G	2505	G1P	O3P-P-O2P	2.19	116.01	107.80
4	C	2540	THM	C5-C4-N3	2.18	117.22	115.32
4	C	2540	THM	C2'-C1'-N1	-2.18	108.37	113.81
2	E	2504	G1P	O1-P-O1P	-2.18	101.57	109.33
4	B	2539	THM	C6-N1-C2	2.17	123.46	121.30
4	B	2539	THM	N3-C2-N1	2.14	117.68	114.89
2	G	2505	G1P	O5-C5-C4	2.14	113.56	109.70
4	C	2532	THM	C2'-C1'-N1	2.14	119.16	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2542	THM	C6-C5-C4	2.14	119.78	118.02
4	A	2538	THM	C3'-C2'-C1'	-2.13	97.39	102.60
4	G	2544	THM	C6-C5-C4	2.12	119.76	118.02
2	D	2503	G1P	C6-C5-C4	2.11	118.19	113.02
2	D	2503	G1P	O3P-P-O1	2.10	114.05	105.85
2	C	2502	G1P	O1-C1-C2	-2.09	104.54	108.38
4	E	2534	THM	O4'-C1'-C2'	-2.06	102.40	106.25
3	A	2507	SO4	O3-S-O2	2.06	120.31	109.56
3	C	2509	SO4	O4-S-O1	-2.02	99.01	109.56
4	B	2539	THM	O4'-C4'-C3'	-2.01	101.08	105.65
2	D	2503	G1P	O2-C2-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2534	THM	O4'-C4'-C5'-O5'
2	C	2502	G1P	O5-C5-C6-O6
4	H	2537	THM	O4'-C4'-C5'-O5'
2	H	2506	G1P	O5-C5-C6-O6
4	D	2533	THM	O4'-C4'-C5'-O5'
4	E	2534	THM	C3'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 26 short contacts:

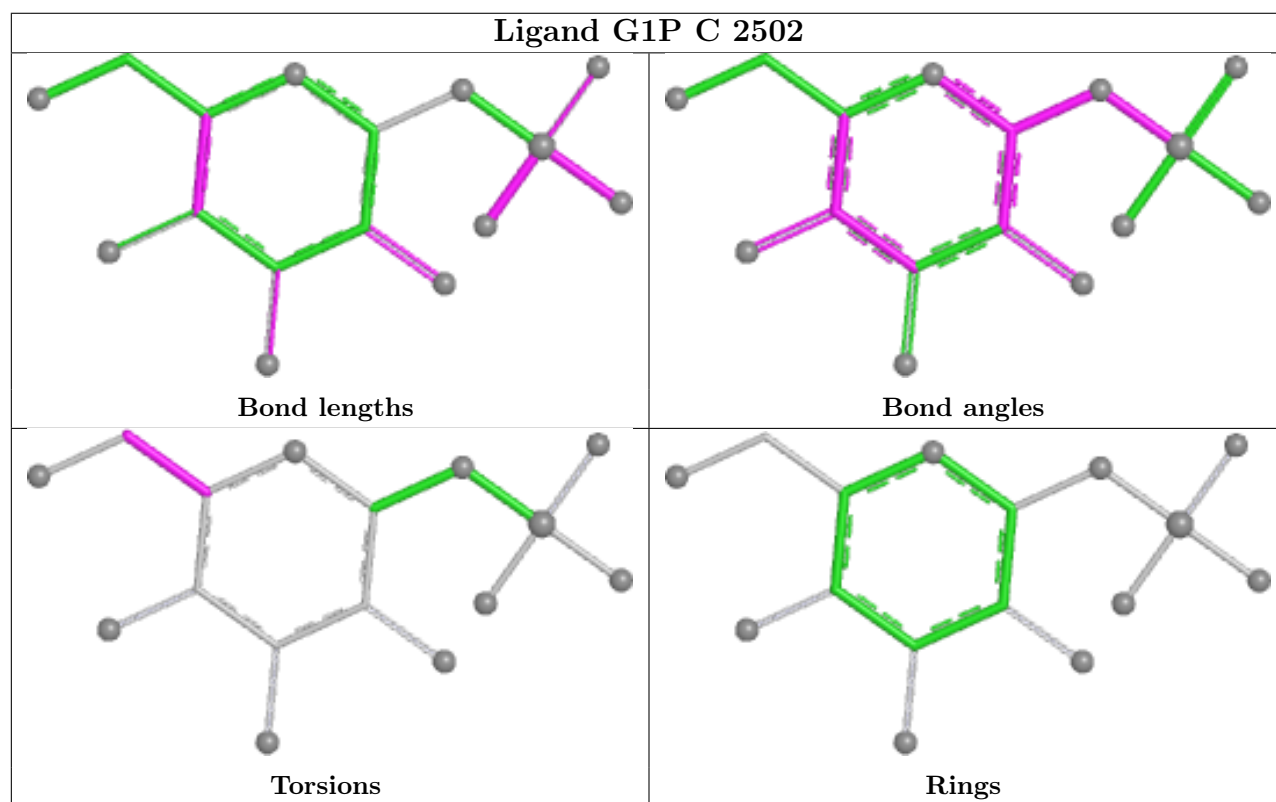
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2502	G1P	2	0
2	B	2501	G1P	2	0
4	H	2537	THM	2	0
2	A	2500	G1P	2	0
2	E	2504	G1P	3	0
4	A	2530	THM	1	0
3	E	2520	SO4	1	0
3	H	2518	SO4	1	0
3	A	2507	SO4	3	0
2	G	2505	G1P	1	0
2	H	2506	G1P	1	0
3	H	2526	SO4	1	0
2	D	2503	G1P	2	0
4	F	2535	THM	2	0

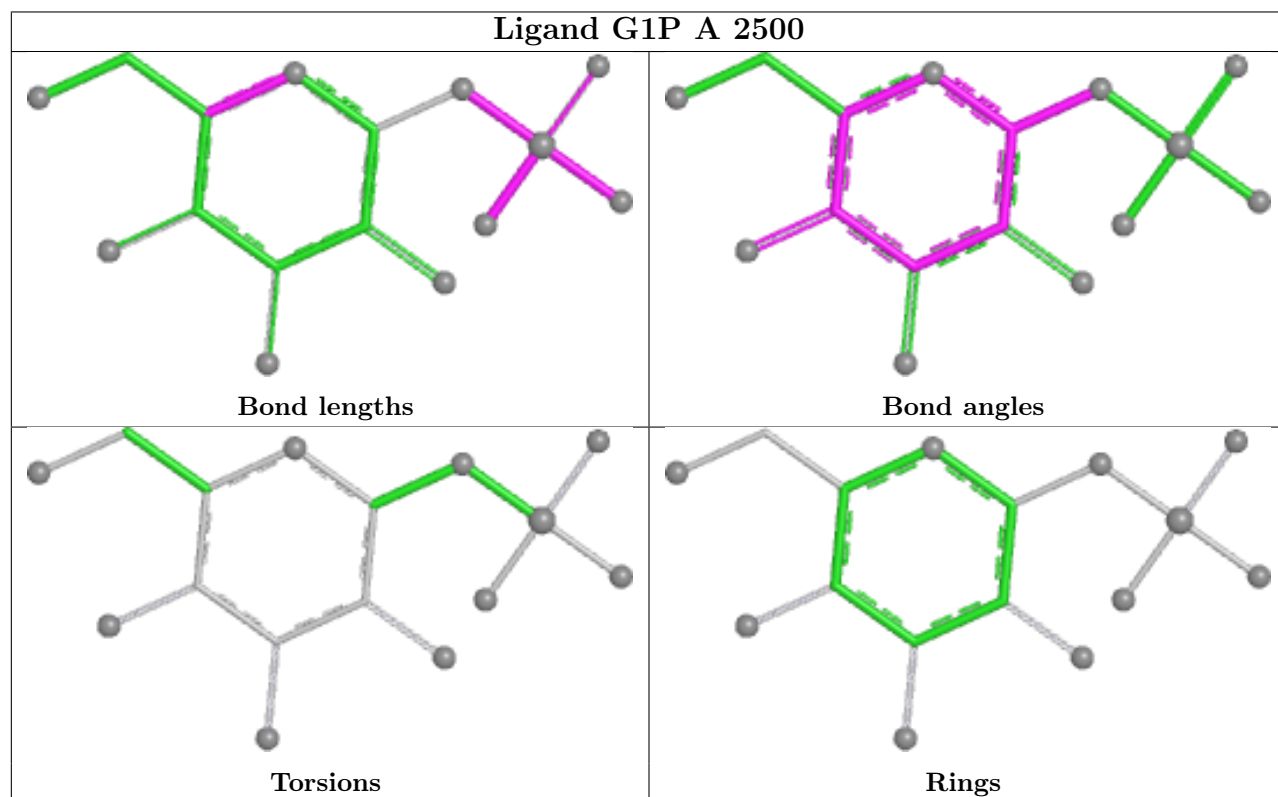
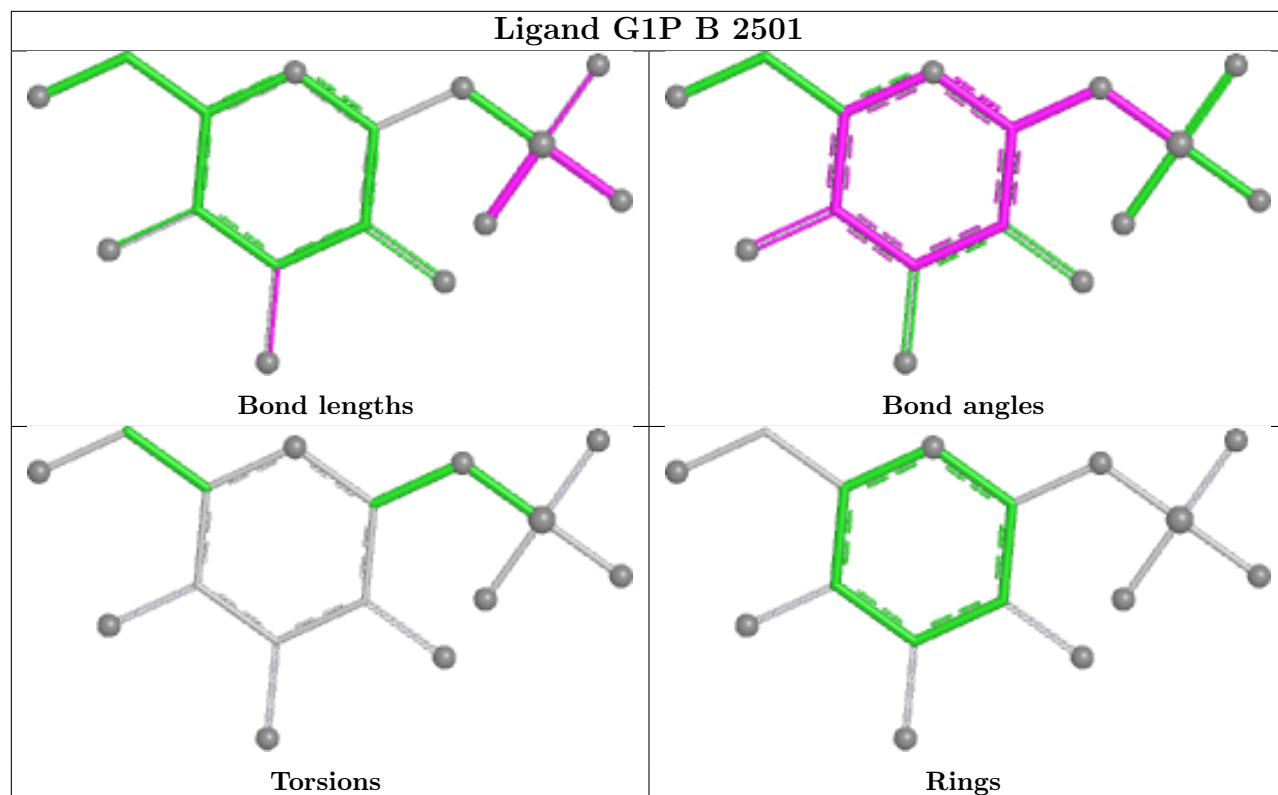
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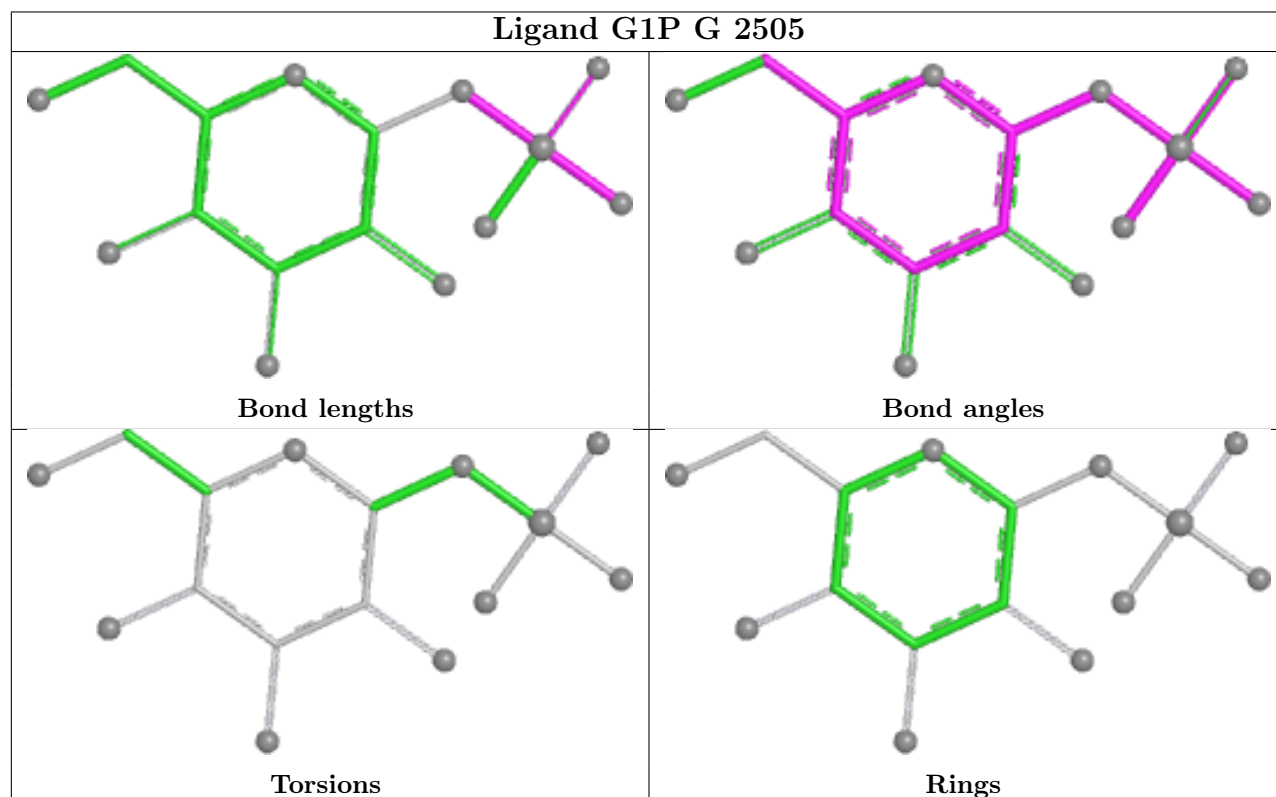
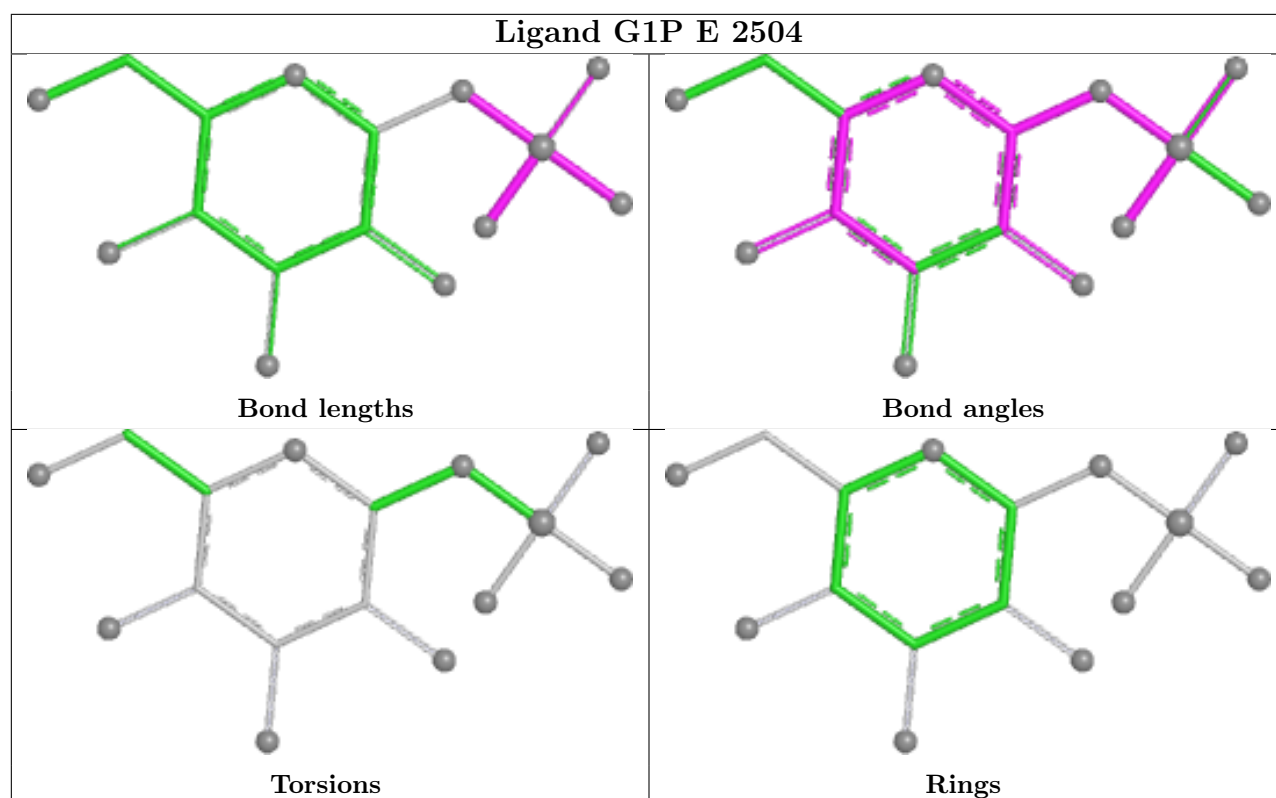
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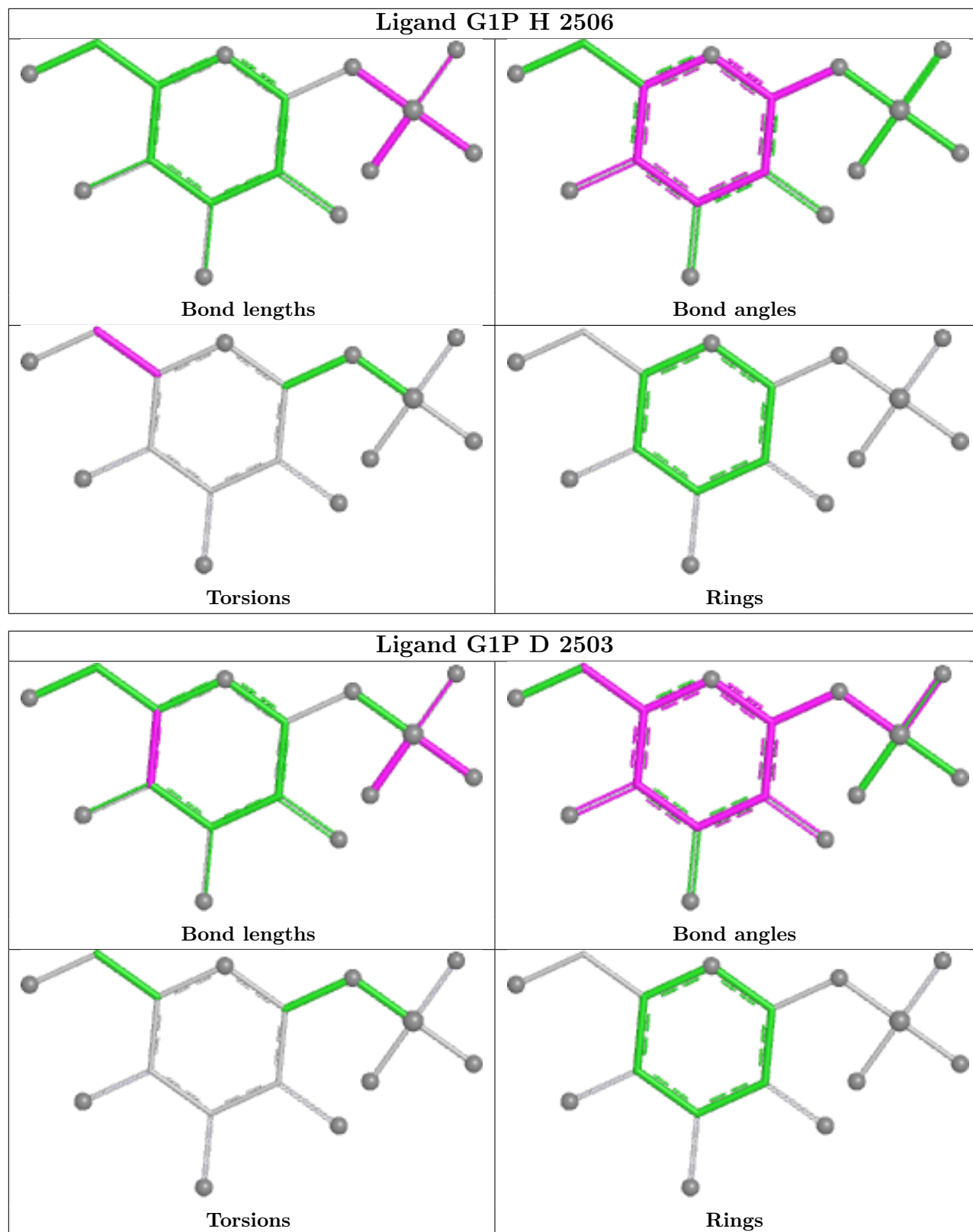
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2524	SO4	1	0
4	G	2536	THM	1	0

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









5.7 Other polymers ⓘ

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, 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	292/293 (99%)	-0.39	1 (0%) 90 93	6, 16, 31, 40	6 (2%)
1	B	292/293 (99%)	-0.47	1 (0%) 90 93	5, 14, 27, 34	8 (2%)
1	C	292/293 (99%)	-0.33	3 (1%) 79 83	6, 16, 32, 49	5 (1%)
1	D	292/293 (99%)	-0.19	6 (2%) 63 70	6, 18, 36, 57	5 (1%)
1	E	292/293 (99%)	0.07	8 (2%) 56 61	7, 22, 42, 63	4 (1%)
1	F	293/293 (100%)	-0.34	5 (1%) 69 74	5, 14, 33, 56	5 (1%)
1	G	292/293 (99%)	-0.53	0 100 100	4, 13, 26, 42	5 (1%)
1	H	292/293 (99%)	-0.34	0 100 100	7, 18, 30, 43	2 (0%)
All	All	2337/2344 (99%)	-0.31	24 (1%) 79 83	4, 16, 33, 63	40 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	5.8
1	C	13	GLY	5.7
1	E	14	THR	5.2
1	F	13	GLY	5.1
1	D	13	GLY	4.6
1	F	14	THR	4.6
1	C	14	THR	4.4
1	E	13	GLY	4.3
1	A	22	ALA	4.0
1	D	16	LEU	3.4
1	D	14	THR	3.1
1	E	195	GLY	3.0
1	E	193	PRO	2.9
1	F	119	HIS	2.7
1	F	23	ILE	2.6
1	D	23	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	16	LEU	2.4
1	E	60	THR	2.3
1	F	16	LEU	2.2
1	E	12	SER	2.2
1	E	15	ARG	2.2
1	D	15	ARG	2.1
1	B	22	ALA	2.0
1	E	23	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	SO4	A	2507	5/5	0.75	0.12	45,47,50,52	0
4	THM	E	2534	17/17	0.82	0.14	39,45,50,55	0
3	SO4	H	2529	5/5	0.84	0.11	45,45,50,51	0
3	SO4	B	2510	5/5	0.85	0.10	40,48,51,53	0
3	SO4	G	2525	5/5	0.85	0.12	45,46,47,52	0
3	SO4	F	2519	5/5	0.86	0.10	55,56,57,60	0
2	G1P	E	2504	16/16	0.87	0.10	34,47,56,59	0
2	G1P	B	2501	16/16	0.88	0.11	29,40,44,45	0
4	THM	F	2535	17/17	0.89	0.11	22,30,44,47	0
3	SO4	E	2520	5/5	0.90	0.09	45,46,52,56	0
2	G1P	C	2502	16/16	0.91	0.09	30,42,48,49	0
3	SO4	D	2514	5/5	0.91	0.07	48,50,51,52	0
4	THM	D	2533	17/17	0.93	0.08	27,30,35,37	0
2	G1P	D	2503	16/16	0.93	0.08	30,37,41,42	0
4	THM	E	2542	17/17	0.93	0.08	26,30,32,32	0

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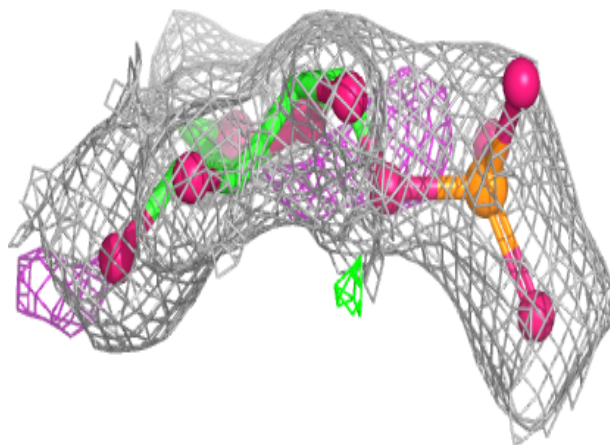
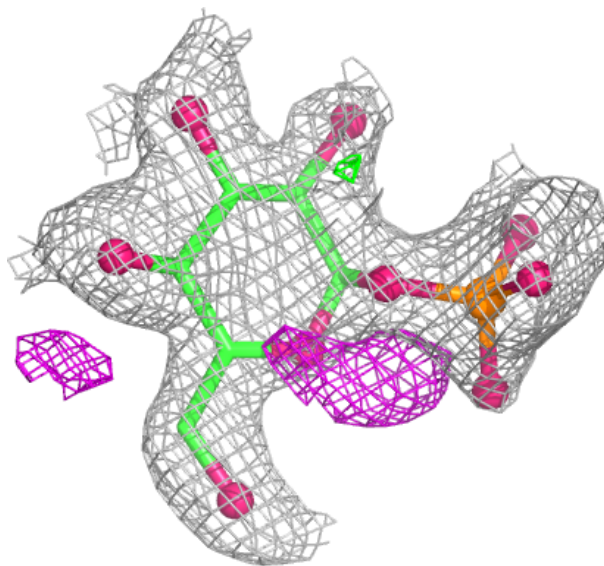
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	F	2522	5/5	0.93	0.08	39,45,48,53	0
4	THM	B	2539	17/17	0.94	0.07	21,24,25,28	0
4	THM	C	2532	17/17	0.94	0.08	24,30,38,45	0
4	THM	A	2530	17/17	0.94	0.08	24,29,32,38	0
4	THM	H	2545	17/17	0.94	0.08	19,25,27,31	0
2	G1P	G	2505	16/16	0.95	0.08	26,32,37,38	0
4	THM	B	2531	17/17	0.95	0.07	19,24,33,35	0
2	G1P	H	2506	16/16	0.95	0.07	29,34,41,42	0
3	SO4	C	2515	5/5	0.95	0.06	40,48,51,52	0
4	THM	F	2543	17/17	0.95	0.07	19,23,26,27	0
4	THM	G	2536	17/17	0.95	0.07	20,24,29,29	0
4	THM	G	2544	17/17	0.95	0.07	17,22,25,27	0
4	THM	H	2537	17/17	0.95	0.08	20,26,33,39	0
4	THM	C	2540	17/17	0.95	0.07	20,22,25,26	0
3	SO4	D	2512	5/5	0.96	0.11	38,42,43,45	0
4	THM	A	2538	17/17	0.96	0.06	19,22,25,27	0
3	SO4	B	2528	5/5	0.96	0.08	39,41,43,43	0
3	SO4	F	2524	5/5	0.96	0.07	36,38,41,42	0
3	SO4	D	2517	5/5	0.96	0.06	45,48,52,56	0
3	SO4	H	2526	5/5	0.96	0.10	39,41,42,43	0
2	G1P	A	2500	16/16	0.96	0.06	28,30,40,40	0
4	THM	D	2541	17/17	0.96	0.06	19,21,24,24	0
3	SO4	C	2509	5/5	0.97	0.07	31,37,40,45	0
3	SO4	F	2521	5/5	0.98	0.04	19,20,23,26	0
3	SO4	H	2518	5/5	0.98	0.05	24,24,26,26	0
3	SO4	E	2527	5/5	0.98	0.05	22,23,24,26	0
3	SO4	C	2513	5/5	0.98	0.05	21,22,24,25	0
3	SO4	B	2511	5/5	0.99	0.05	20,21,26,26	0
3	SO4	D	2516	5/5	0.99	0.04	18,22,23,25	0
3	SO4	A	2508	5/5	0.99	0.06	22,23,24,24	0
3	SO4	G	2523	5/5	0.99	0.04	19,20,23,27	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.

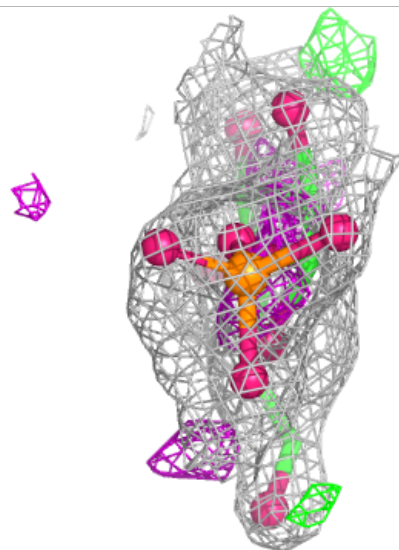
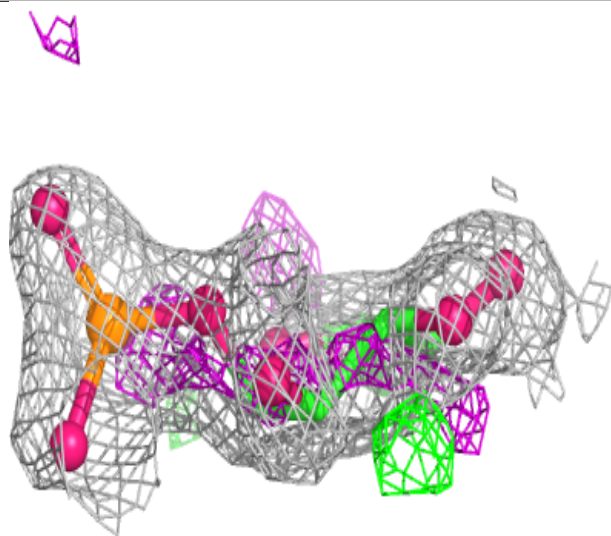
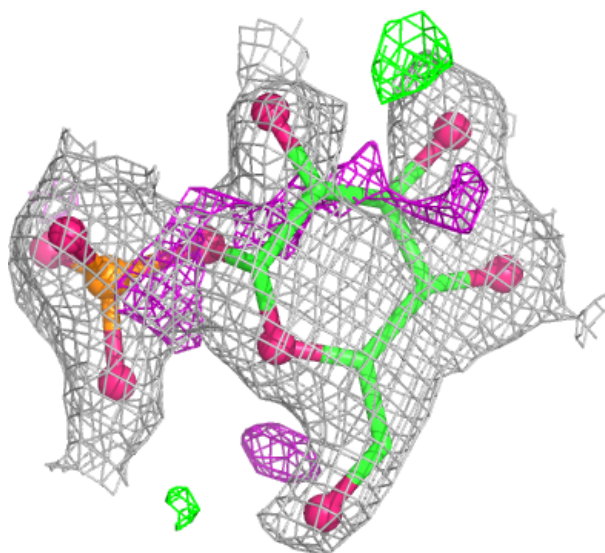
Electron density around G1P E 2504:

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



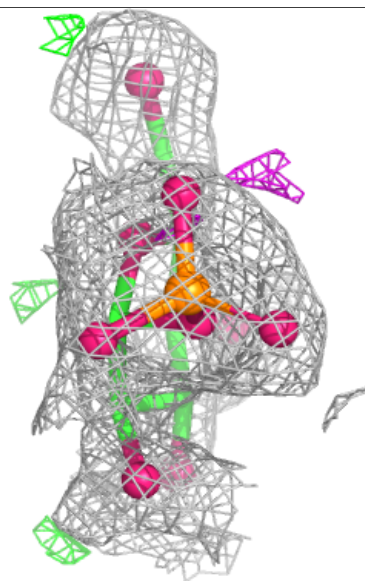
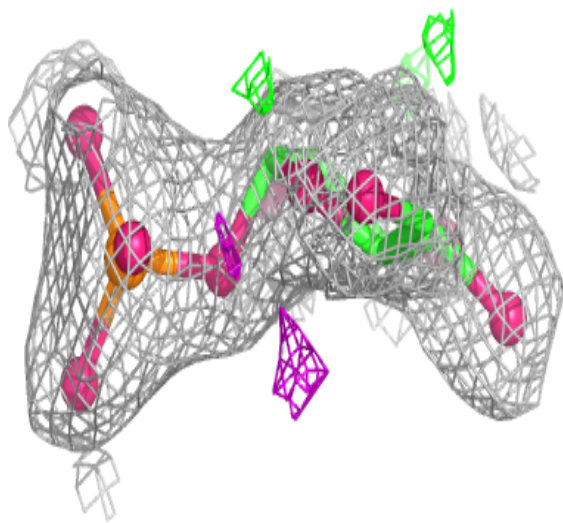
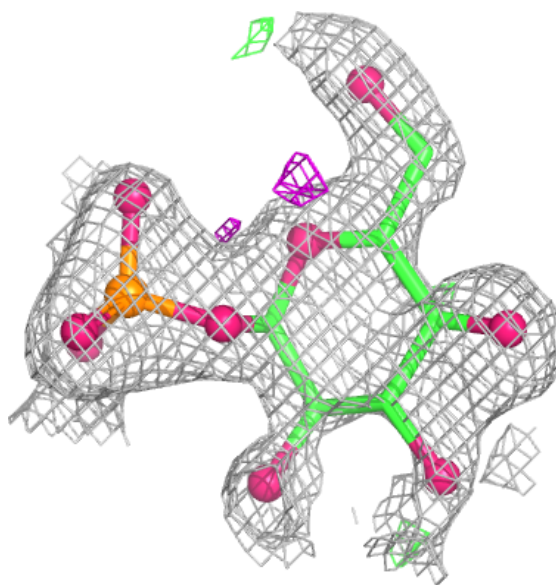
Electron density around G1P B 2501:

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



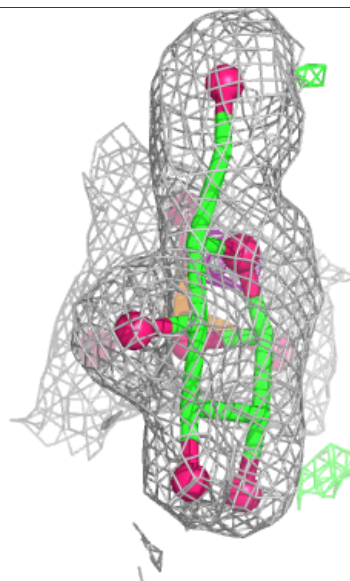
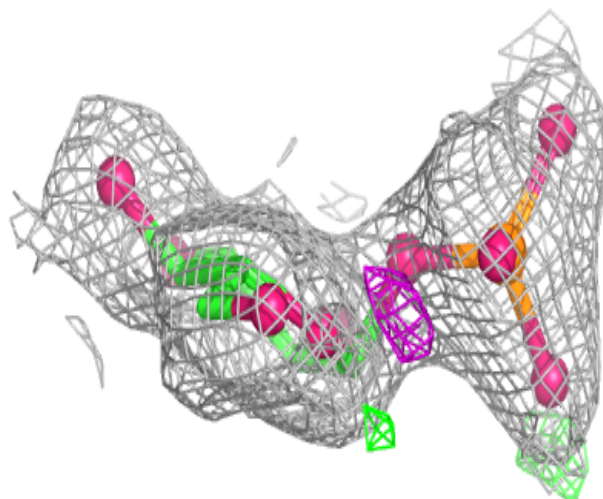
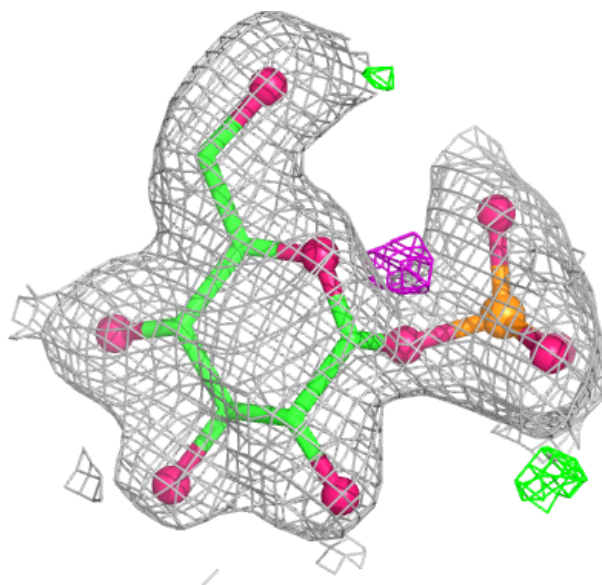
Electron density around G1P C 2502:

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



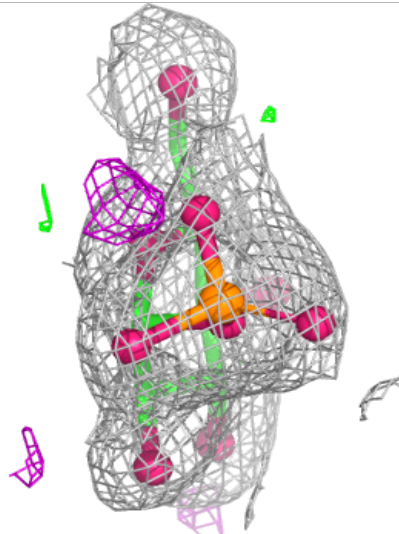
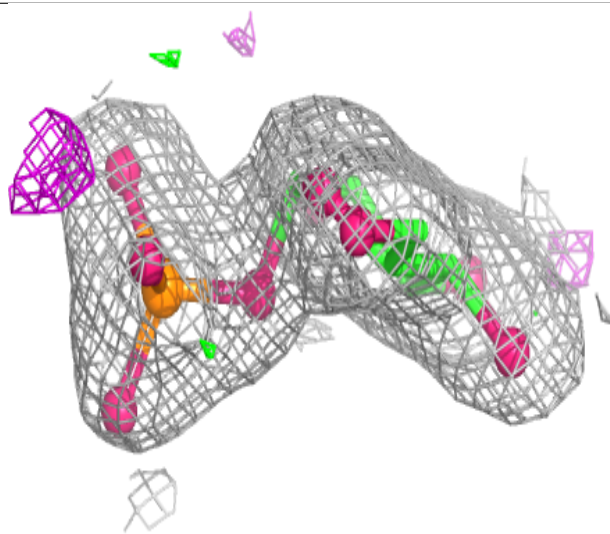
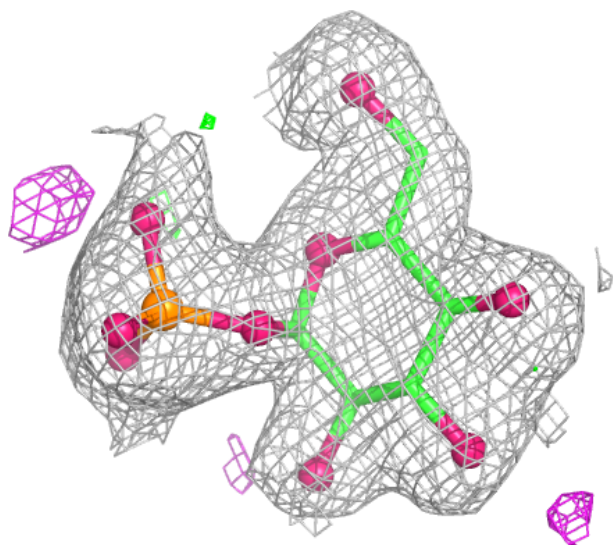
Electron density around G1P D 2503:

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



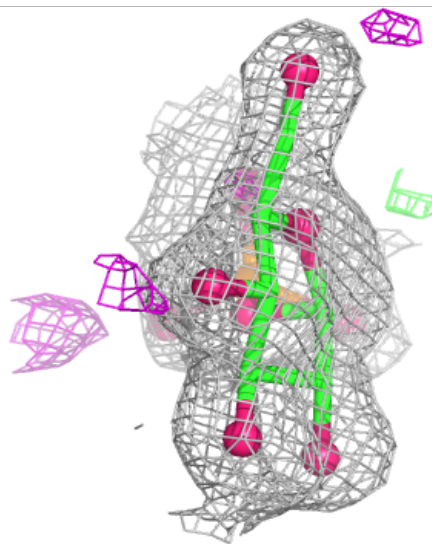
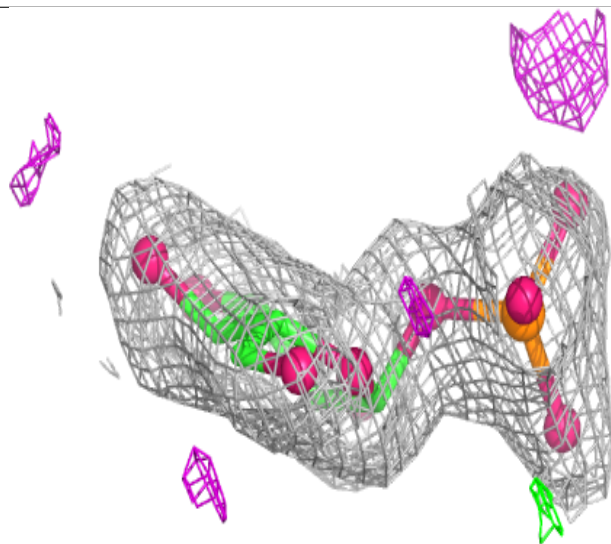
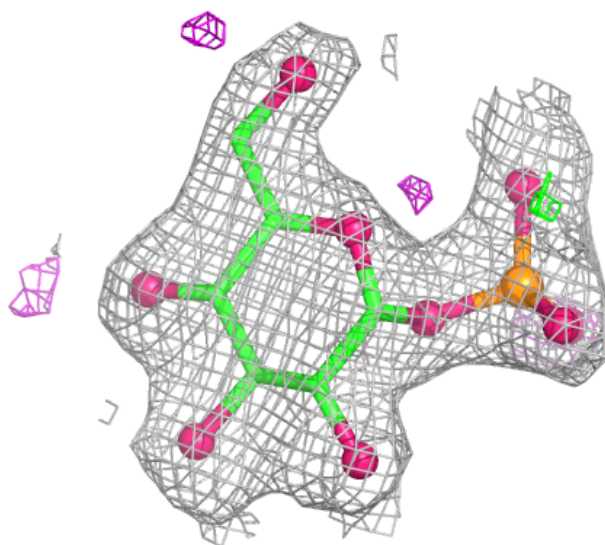
Electron density around G1P G 2505:

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



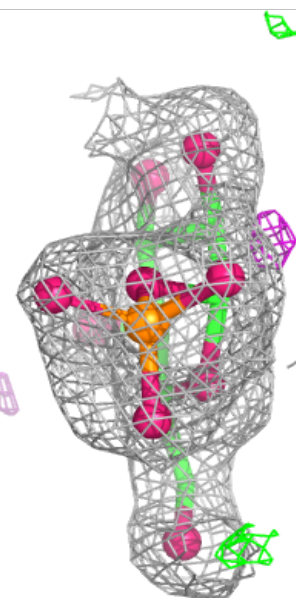
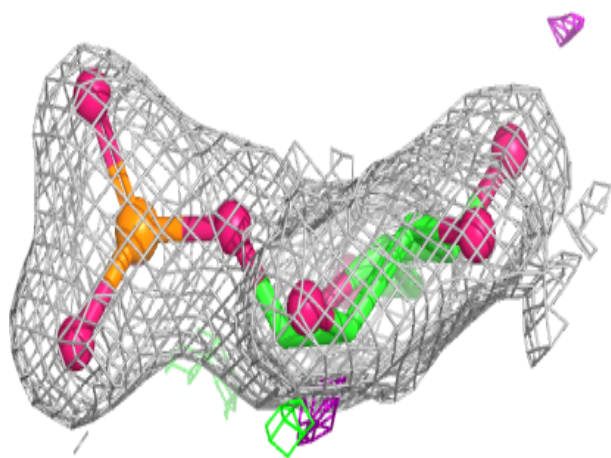
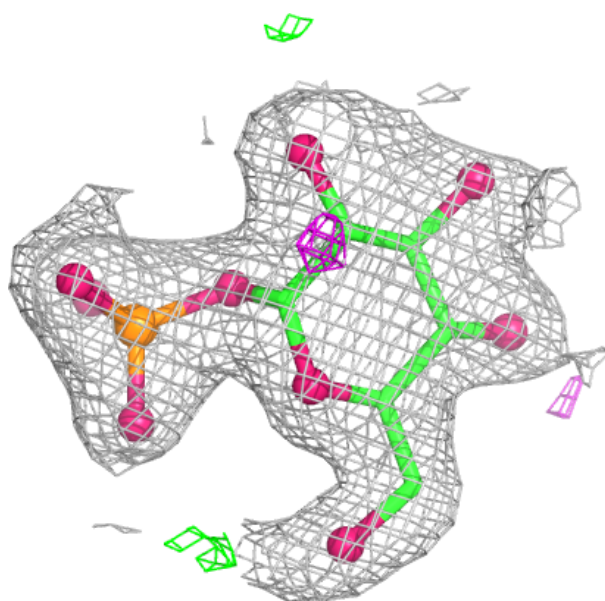
Electron density around G1P H 2506:

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



Electron density around G1P A 2500:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.