Full wwPDB X-ray Structure Validation Report (i)

Nov 24, 2025 – 12:16 PM EST

PDB ID	:	9ZAX / pdb_00009zax
Title	:	Crystal structure of Phosphoglycerate mutase from Trichomonas vaginalis in complex with 3-phosphoglyceric acid
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2025-11-19
Resolution	:	2.10 Å(reported)

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

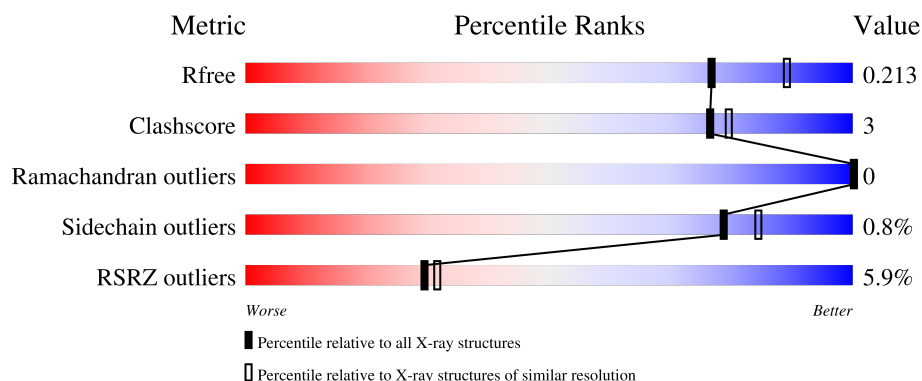|		
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.213
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		5.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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 <=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	258	5% / 83% / 7% / 11%
1	B	258	3% / 81% / 7% / 12%
1	C	258	8% / 82% / 5% / 13%
1	D	258	5% / 82% / • / 14%

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	3PG	A	302	-	-	X	-
3	3PG	B	301	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7786 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 Phosphoglycerate mutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	P	S	0	1	0
			1846	1174	312	344	1	15			
1	B	228	Total	C	N	O	P	S	0	2	0
			1841	1173	310	342	1	15			
1	C	224	Total	C	N	O	P	S	0	0	0
			1761	1120	300	326	1	14			
1	D	222	Total	C	N	O	P	S	0	0	0
			1744	1106	297	326	1	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A2DUN8
A	-6	ALA	-	expression tag	UNP A2DUN8
A	-5	HIS	-	expression tag	UNP A2DUN8
A	-4	HIS	-	expression tag	UNP A2DUN8
A	-3	HIS	-	expression tag	UNP A2DUN8
A	-2	HIS	-	expression tag	UNP A2DUN8
A	-1	HIS	-	expression tag	UNP A2DUN8
A	0	HIS	-	expression tag	UNP A2DUN8
B	-7	MET	-	expression tag	UNP A2DUN8
B	-6	ALA	-	expression tag	UNP A2DUN8
B	-5	HIS	-	expression tag	UNP A2DUN8
B	-4	HIS	-	expression tag	UNP A2DUN8
B	-3	HIS	-	expression tag	UNP A2DUN8
B	-2	HIS	-	expression tag	UNP A2DUN8
B	-1	HIS	-	expression tag	UNP A2DUN8
B	0	HIS	-	expression tag	UNP A2DUN8
C	-7	MET	-	expression tag	UNP A2DUN8
C	-6	ALA	-	expression tag	UNP A2DUN8
C	-5	HIS	-	expression tag	UNP A2DUN8
C	-4	HIS	-	expression tag	UNP A2DUN8
C	-3	HIS	-	expression tag	UNP A2DUN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP A2DUN8
C	-1	HIS	-	expression tag	UNP A2DUN8
C	0	HIS	-	expression tag	UNP A2DUN8
D	-7	MET	-	expression tag	UNP A2DUN8
D	-6	ALA	-	expression tag	UNP A2DUN8
D	-5	HIS	-	expression tag	UNP A2DUN8
D	-4	HIS	-	expression tag	UNP A2DUN8
D	-3	HIS	-	expression tag	UNP A2DUN8
D	-2	HIS	-	expression tag	UNP A2DUN8
D	-1	HIS	-	expression tag	UNP A2DUN8
D	0	HIS	-	expression tag	UNP A2DUN8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total Cl 1 1		0	0

- Molecule 3 is 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: $C_3H_7O_7P$) (labeled as "Ligand of Interest" by depositor).
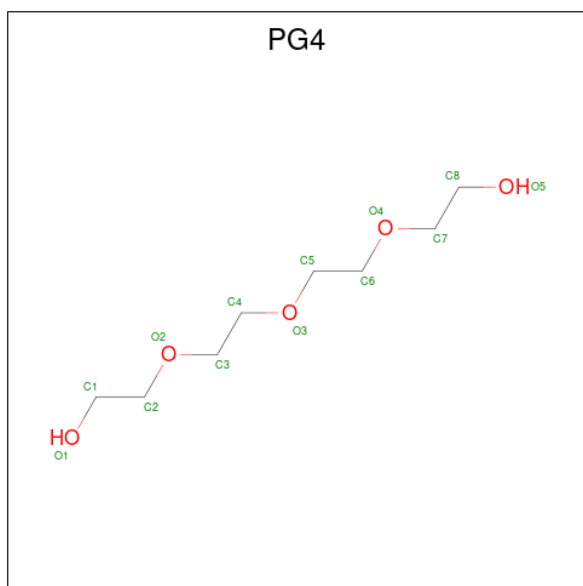

3PG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total C O P 11 3 7 1				0	0
3	B	1	Total C O P 11 3 7 1				0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 11	C 3	O 7	P 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 8	O 5	0	0
4	A	1	Total 6	C 4	O 2	0	0
4	A	1	Total 10	C 6	O 4	0	0
4	B	1	Total 7	C 4	O 3	0	0
4	B	1	Total 7	C 4	O 3	0	0
4	B	1	Total 7	C 4	O 3	0	0
4	B	1	Total 9	C 6	O 3	0	0
4	C	1	Total 7	C 4	O 3	0	0
4	C	1	Total 7	C 4	O 3	0	0
4	D	1	Total 7	C 4	O 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

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

- Molecule 6 is water.

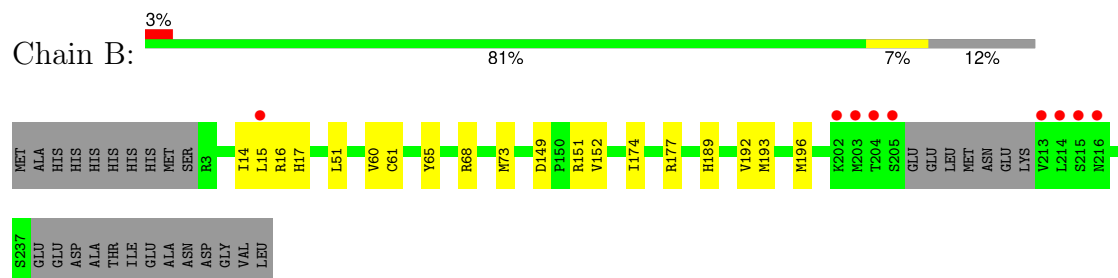| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	159	Total 159	O 159	0	0
6	B	136	Total 136	O 136	0	0
6	C	66	Total 66	O 66	0	0
6	D	94	Total 94	O 94	0	0

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.

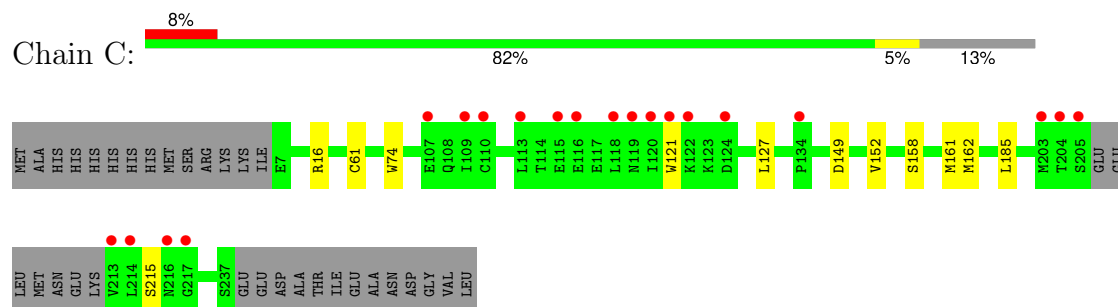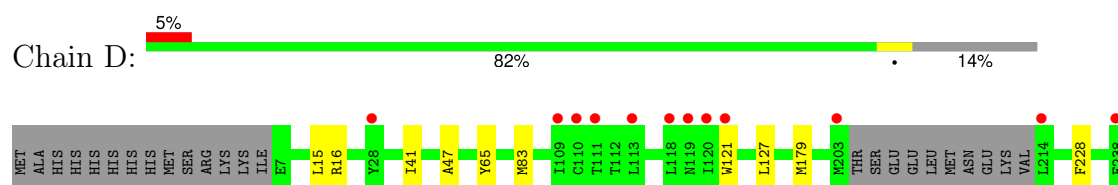- Molecule 1: Phosphoglycerate mutase

Chain A:

- Molecule 1: Phosphoglycerate mutase

Chain B:

- Molecule 1: Phosphoglycerate mutase

Chain C:

- Molecule 1: Phosphoglycerate mutase

Chain D:

GLU ASP ALA THR ILE GLU ALA ASN ASP GLY VAL LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.64Å 93.06Å 95.48Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	48.83 – 2.10 48.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.83-2.10) 99.7 (48.83-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.10Å)	Xtriage
Refinement program	PHENIX (2.0_5882: ???)	Depositor
R, R_{free}	0.178 , 0.213 0.184 , 0.213	Depositor DCC
R_{free} test set	3501 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.1	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.009 for -h,-l,-k 0.057 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3PG, SO4, PG4, RPI, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.20	0/1874	0.40	0/2532
1	B	0.21	0/1872	0.39	0/2529
1	C	0.17	0/1786	0.36	0/2421
1	D	0.17	0/1769	0.37	0/2398
All	All	0.19	0/7301	0.38	0/9880

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1846	0	1803	16	0
1	B	1841	0	1810	14	0
1	C	1761	0	1679	6	0
1	D	1744	0	1642	5	0
2	A	1	0	0	0	0
3	A	11	0	4	8	0
3	B	11	0	4	6	0
3	D	11	0	4	0	0
4	A	29	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	33	0	0
4	C	14	0	17	0	0
4	D	7	0	9	1	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	A	159	0	0	1	0
6	B	136	0	0	0	0
6	C	66	0	0	0	0
6	D	94	0	0	0	0
All	All	7786	0	7042	40	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 3.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HE	3:A:302:3PG:H31	1.35	0.90
1:A:68:ARG:NE	3:A:302:3PG:H31	2.03	0.72
1:A:17:HIS:CE1	3:A:302:3PG:H32	2.26	0.70
1:B:17:HIS:CE1	3:B:301:3PG:H32	2.27	0.69
1:A:123:LYS:HG3	1:A:124:ASP:OD2	1.92	0.69
1:A:26:ARG:NH2	6:A:401:HOH:O	2.28	0.67
1:B:68:ARG:HH21	3:B:301:3PG:H31	1.58	0.66
1:B:14:ILE:HG22	1:B:193:MET:HE2	1.81	0.62
1:A:68:ARG:HH21	3:A:302:3PG:H31	1.67	0.60
1:B:149:ASP:O	1:B:152:VAL:HG12	2.05	0.57
1:D:41:ILE:HD11	4:D:302:PG4:H81	1.87	0.56
1:B:15:LEU:HD12	1:B:51:LEU:HD11	1.87	0.56
1:C:74:TRP:CZ3	1:D:83:MET:HE3	2.42	0.55
1:C:149:ASP:O	1:C:152:VAL:HG12	2.06	0.55
1:B:189:HIS:HB3	3:B:301:3PG:O3	2.07	0.53
1:A:101:LEU:HD22	1:A:129:PRO:HB3	1.90	0.53
1:B:149:ASP:OD1	1:B:151:ARG:HD2	2.10	0.52
1:B:17:HIS:NE2	3:B:301:3PG:H32	2.25	0.51
1:A:68:ARG:NH2	3:A:302:3PG:H31	2.26	0.50
1:B:68:ARG:HE	3:B:301:3PG:H31	1.76	0.50
1:B:61:CYS:SG	1:B:73:MET:HG3	2.52	0.49
1:C:158:SER:OG	1:C:161:MET:HG3	2.14	0.48
1:A:68:ARG:HE	3:A:302:3PG:C3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:HIS:HE1	3:A:302:3PG:H32	1.78	0.46
1:B:68:ARG:HE	3:B:301:3PG:C3	2.28	0.46
1:C:121:TRP:HB2	1:C:127:LEU:HD22	1.99	0.45
1:B:192:VAL:HG12	1:B:196:MET:HE3	1.99	0.44
1:D:121:TRP:HB2	1:D:127:LEU:HD23	1.98	0.44
1:A:162:MET:SD	1:A:162:MET:C	3.02	0.43
1:A:118:LEU:O	1:A:122:LYS:HG3	2.19	0.43
1:D:179:MET:CE	1:D:228:PHE:HB2	2.49	0.42
1:A:68:ARG:CZ	3:A:302:3PG:H31	2.48	0.42
1:A:123:LYS:CG	1:A:124:ASP:OD2	2.63	0.42
1:C:61:CYS:SG	1:C:185:LEU:HD23	2.60	0.42
1:D:15:LEU:HD11	1:D:47:ALA:HB1	2.02	0.41
1:A:66:LEU:HD12	1:A:189:HIS:CE1	2.56	0.41
1:B:60:VAL:HG11	1:B:177:ARG:HD3	2.02	0.41
1:B:149:ASP:CG	1:B:151:ARG:HD2	2.46	0.41
1:C:162:MET:C	1:C:162:MET:SD	3.04	0.41
1:A:149:ASP:O	1:A:152:VAL:HG12	2.22	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	226/258 (88%)	220 (97%)	6 (3%)	0	100	100
1	B	225/258 (87%)	221 (98%)	4 (2%)	0	100	100
1	C	219/258 (85%)	216 (99%)	3 (1%)	0	100	100
1	D	217/258 (84%)	212 (98%)	5 (2%)	0	100	100
All	All	887/1032 (86%)	869 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	203/233 (87%)	201 (99%)	2 (1%)	73	79
1	B	204/233 (88%)	202 (99%)	2 (1%)	73	79
1	C	187/233 (80%)	186 (100%)	1 (0%)	86	91
1	D	184/233 (79%)	183 (100%)	1 (0%)	86	91
All	All	778/932 (84%)	772 (99%)	6 (1%)	79	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	TYR
1	A	174	ILE
1	B	65	TYR
1	B	174	ILE
1	C	215	SER
1	D	65	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	C	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\#|Z| > 2$
1	RPI	B	16	1	11,14,15	1.69	4 (36%)	10,18,20	1.20	2 (20%)
1	RPI	D	16	1	11,14,15	1.80	5 (45%)	10,18,20	1.02	0
1	RPI	C	16	1	11,14,15	1.78	5 (45%)	10,18,20	0.98	0
1	RPI	A	16	1	11,14,15	1.75	5 (45%)	10,18,20	1.07	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
1	RPI	B	16	1	-	6/9/14/16	-
1	RPI	D	16	1	-	7/9/14/16	-
1	RPI	C	16	1	-	6/9/14/16	-
1	RPI	A	16	1	-	6/9/14/16	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	16	RPI	P-O2P	3.20	1.51	1.46
1	D	16	RPI	P-NH2	2.93	1.68	1.63
1	A	16	RPI	P-O2P	2.91	1.50	1.46
1	C	16	RPI	P-O2P	2.90	1.50	1.46
1	C	16	RPI	P-NH2	2.81	1.68	1.63
1	B	16	RPI	P-O2P	2.76	1.50	1.46
1	B	16	RPI	CZ-NH2	-2.76	1.32	1.36
1	A	16	RPI	CZ-NH2	-2.66	1.33	1.36
1	C	16	RPI	CZ-NH2	-2.57	1.33	1.36
1	B	16	RPI	P-O1P	-2.44	1.50	1.56
1	A	16	RPI	P-O1P	-2.42	1.50	1.56
1	C	16	RPI	P-O1P	-2.38	1.50	1.56
1	A	16	RPI	P-O3P	-2.37	1.50	1.56
1	D	16	RPI	CZ-NH2	-2.36	1.33	1.36
1	C	16	RPI	P-O3P	-2.36	1.50	1.56
1	B	16	RPI	P-O3P	-2.35	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	RPI	P-NH2	2.32	1.67	1.63
1	D	16	RPI	P-O3P	-2.30	1.50	1.56
1	D	16	RPI	P-O1P	-2.26	1.50	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	RPI	O3P-P-O2P	-2.21	107.91	113.45
1	B	16	RPI	O2P-P-NH2	-2.10	107.67	111.03

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	RPI	CZ-NH2-P-O2P
1	A	16	RPI	C-CA-CB-CG
1	A	16	RPI	O-C-CA-CB
1	A	16	RPI	NH1-CZ-NE-CD
1	A	16	RPI	NH2-CZ-NE-CD
1	B	16	RPI	CZ-NH2-P-O2P
1	B	16	RPI	N-CA-CB-CG
1	B	16	RPI	C-CA-CB-CG
1	B	16	RPI	NH1-CZ-NE-CD
1	B	16	RPI	NH2-CZ-NE-CD
1	C	16	RPI	CZ-NH2-P-O2P
1	C	16	RPI	N-CA-CB-CG
1	C	16	RPI	C-CA-CB-CG
1	C	16	RPI	NH1-CZ-NE-CD
1	C	16	RPI	NH2-CZ-NE-CD
1	D	16	RPI	CZ-NH2-P-O2P
1	D	16	RPI	N-CA-CB-CG
1	D	16	RPI	C-CA-CB-CG
1	D	16	RPI	O-C-CA-CB
1	D	16	RPI	NE-CD-CG-CB
1	B	16	RPI	NE-CD-CG-CB
1	D	16	RPI	NH2-CZ-NE-CD
1	A	16	RPI	N-CA-CB-CG
1	D	16	RPI	NH1-CZ-NE-CD
1	C	16	RPI	NE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	PG4	C	301	-	6,6,12	0.27	0	5,5,11	0.28	0
5	SO4	D	304	-	4,4,4	0.68	0	6,6,6	0.19	0
4	PG4	B	303	-	6,6,12	0.25	0	5,5,11	0.28	0
5	SO4	B	306	-	4,4,4	0.67	0	6,6,6	0.08	0
3	3PG	A	302	-	9,10,10	0.87	0	11,14,14	1.21	1 (9%)
4	PG4	A	304	-	5,5,12	0.35	0	4,4,11	0.18	0
5	SO4	D	303	-	4,4,4	0.68	0	6,6,6	0.17	0
4	PG4	A	303	-	12,12,12	0.29	0	11,11,11	0.23	0
3	3PG	D	301	-	9,10,10	0.90	0	11,14,14	1.19	2 (18%)
5	SO4	C	303	-	4,4,4	0.71	0	6,6,6	0.23	0
4	PG4	B	302	-	6,6,12	0.29	0	5,5,11	0.28	0
4	PG4	B	305	-	8,8,12	0.26	0	7,7,11	0.17	0
4	PG4	B	304	-	6,6,12	0.26	0	5,5,11	0.25	0
5	SO4	B	307	-	4,4,4	0.68	0	6,6,6	0.10	0
3	3PG	B	301	-	9,10,10	0.85	0	11,14,14	1.27	2 (18%)
4	PG4	A	305	-	9,9,12	0.28	0	8,8,11	0.29	0
4	PG4	D	302	-	6,6,12	0.25	0	5,5,11	0.23	0
4	PG4	C	302	-	6,6,12	0.28	0	5,5,11	0.25	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
4	PG4	C	301	-	-	2/4/4/10	-
4	PG4	B	303	-	-	2/4/4/10	-
3	3PG	A	302	-	-	7/10/10/10	-
4	PG4	A	304	-	-	2/3/3/10	-
4	PG4	A	303	-	-	5/10/10/10	-
3	3PG	D	301	-	-	7/10/10/10	-
4	PG4	B	302	-	-	1/4/4/10	-
4	PG4	B	305	-	-	4/6/6/10	-
4	PG4	B	304	-	-	1/4/4/10	-
3	3PG	B	301	-	-	3/10/10/10	-
4	PG4	A	305	-	-	3/7/7/10	-
4	PG4	D	302	-	-	3/4/4/10	-
4	PG4	C	302	-	-	1/4/4/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	3PG	O1-C1-C2	-2.78	117.04	122.60
3	D	301	3PG	O1-C1-C2	-2.60	117.40	122.60
3	A	302	3PG	O1-C1-C2	-2.41	117.79	122.60
3	B	301	3PG	O2-C1-C2	2.17	117.33	112.74
3	D	301	3PG	O2-C1-C2	2.08	117.15	112.74

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	3PG	C1-C2-C3-O1P
3	A	302	3PG	O3-C2-C3-O1P
3	B	301	3PG	C1-C2-C3-O1P
3	B	301	3PG	O3-C2-C3-O1P
3	D	301	3PG	C2-C3-O1P-P
3	D	301	3PG	C3-O1P-P-O3P
3	D	301	3PG	C3-O1P-P-O4P
4	B	305	PG4	O3-C5-C6-O4
4	D	302	PG4	O3-C5-C6-O4
4	D	302	PG4	O4-C7-C8-O5
4	A	304	PG4	O2-C3-C4-O3
3	A	302	3PG	O1-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
3	A	302	3PG	O2-C1-C2-O3
3	D	301	3PG	O1-C1-C2-O3
3	D	301	3PG	O2-C1-C2-O3
3	D	301	3PG	O2-C1-C2-C3
4	B	304	PG4	O2-C3-C4-O3
4	A	303	PG4	C4-C3-O2-C2
4	A	303	PG4	C3-C4-O3-C5
4	C	302	PG4	C8-C7-O4-C6
4	A	303	PG4	O1-C1-C2-O2
4	B	305	PG4	C6-C5-O3-C4
3	A	302	3PG	C2-C3-O1P-P
4	D	302	PG4	C8-C7-O4-C6
4	A	305	PG4	O2-C3-C4-O3
4	C	301	PG4	O2-C3-C4-O3
3	D	301	3PG	O1-C1-C2-C3
3	B	301	3PG	C2-C3-O1P-P
4	A	304	PG4	C4-C3-O2-C2
4	A	303	PG4	C1-C2-O2-C3
4	A	305	PG4	O3-C5-C6-O4
4	B	303	PG4	C6-C5-O3-C4
4	B	305	PG4	O2-C3-C4-O3
4	A	305	PG4	C6-C5-O3-C4
4	A	303	PG4	O2-C3-C4-O3
4	B	305	PG4	C5-C6-O4-C7
4	B	302	PG4	C6-C5-O3-C4
4	C	301	PG4	O3-C5-C6-O4
4	B	303	PG4	O2-C3-C4-O3
3	A	302	3PG	O1-C1-C2-C3
3	A	302	3PG	O2-C1-C2-C3
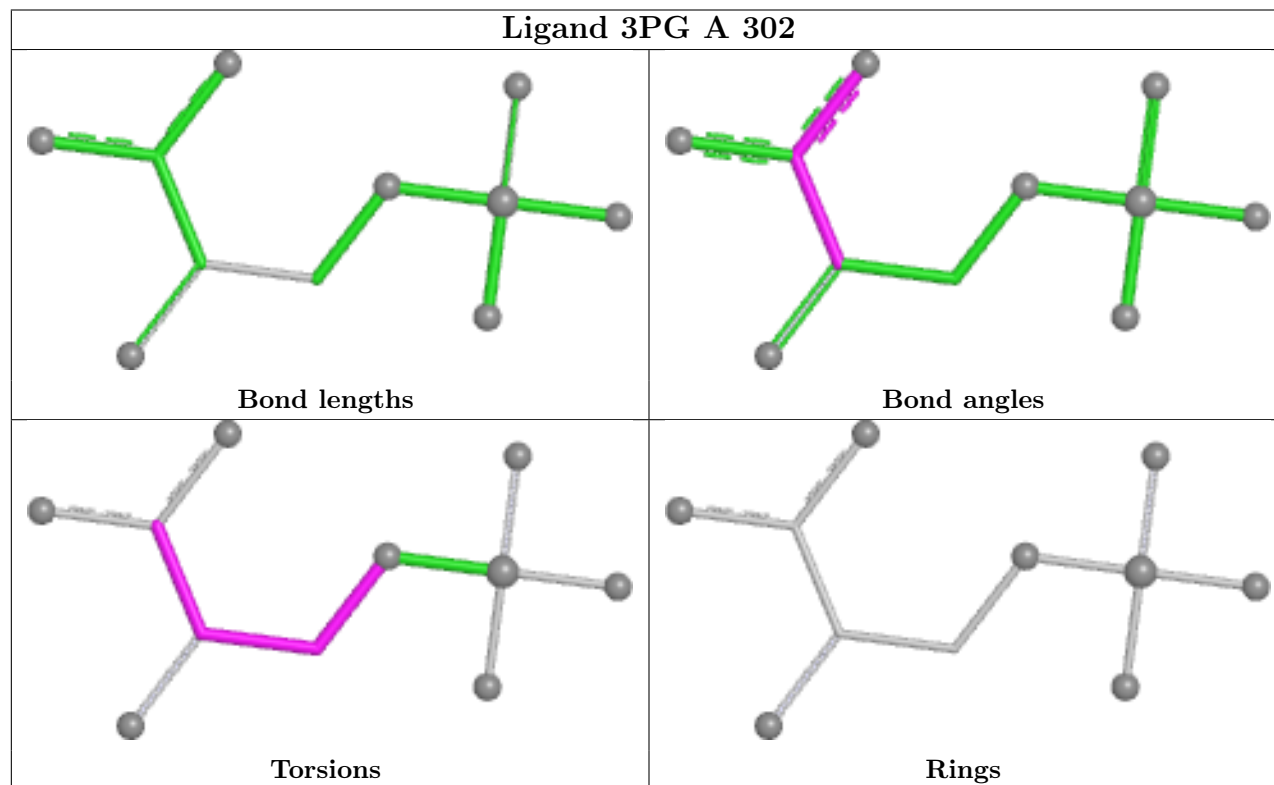
There are no ring outliers.
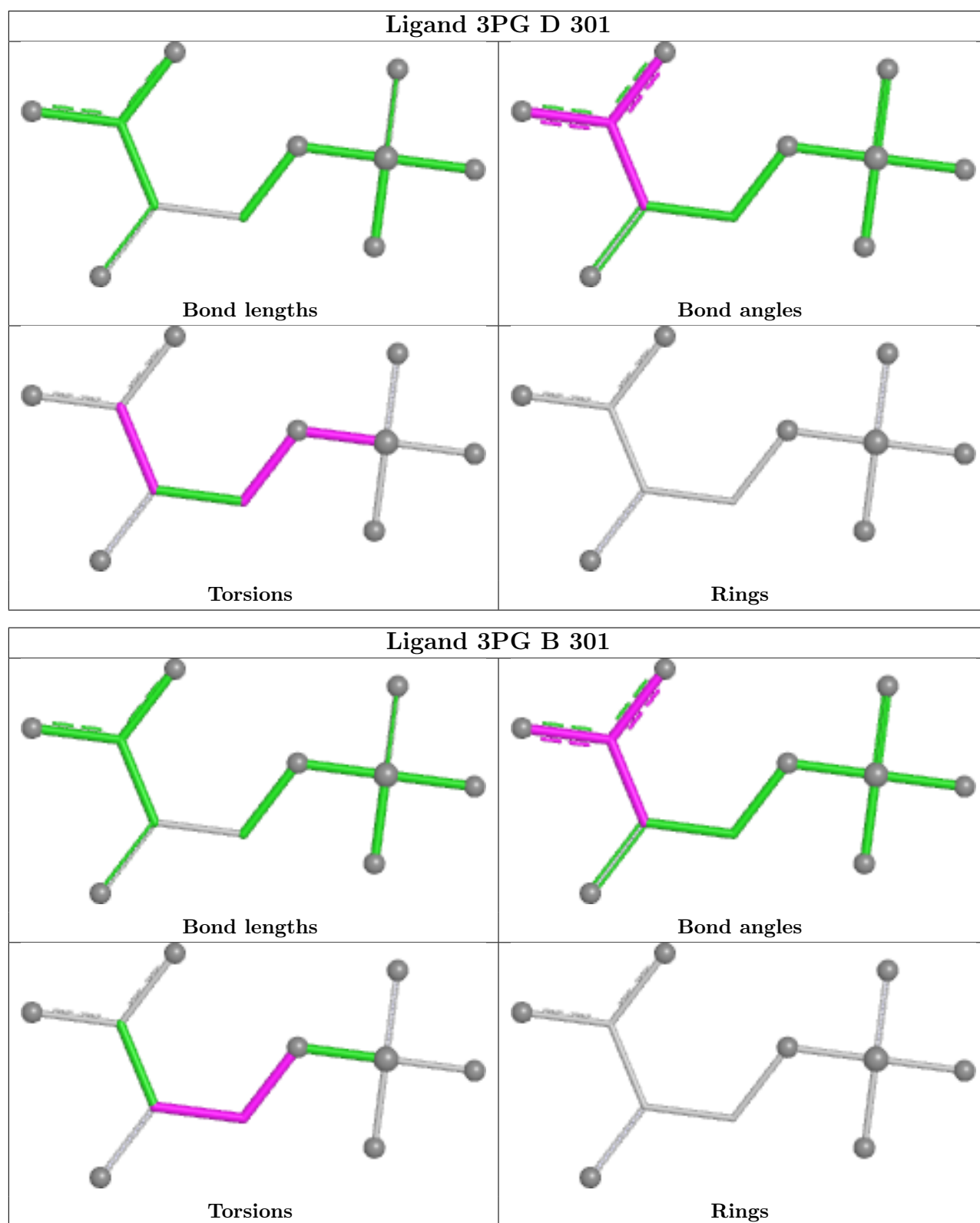
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	3PG	8	0
3	B	301	3PG	6	0
4	D	302	PG4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

Ligand 3PG A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PG D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 3PG B 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	229/258 (88%)	-0.06	12 (5%)	34	36	19, 27, 55, 102	1 (0%)
1	B	227/258 (87%)	-0.09	9 (3%)	43	45	17, 27, 54, 87	2 (0%)
1	C	223/258 (86%)	0.44	20 (8%)	17	18	23, 39, 83, 101	0
1	D	221/258 (85%)	0.29	12 (5%)	32	35	24, 37, 78, 91	0
All	All	900/1032 (87%)	0.14	53 (5%)	29	31	17, 32, 75, 102	3 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	6.0
1	B	213	VAL	4.6
1	B	214	LEU	4.3
1	C	216	ASN	4.3
1	A	204	THR	3.9
1	C	204	THR	3.8
1	D	214	LEU	3.7
1	C	119	ASN	3.7
1	D	118	LEU	3.6
1	C	213	VAL	3.6
1	D	121	TRP	3.6
1	A	203	MET	3.5
1	B	204	THR	3.5
1	C	109	ILE	3.5
1	B	205	SER	3.4
1	B	203	MET	3.4
1	D	110	CYS	3.4
1	C	205	SER	3.4
1	A	215	SER	3.3
1	A	216	ASN	3.2
1	C	121	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	107	GLU	3.2
1	C	110	CYS	3.1
1	D	238	GLU	2.9
1	D	203	MET	2.9
1	C	214	LEU	2.9
1	A	206	GLU	2.8
1	A	3	ARG	2.7
1	C	115	GLU	2.7
1	B	15	LEU	2.7
1	B	216	ASN	2.6
1	D	113	LEU	2.6
1	C	116	GLU	2.6
1	D	119	ASN	2.6
1	A	207	GLU	2.6
1	A	205	SER	2.5
1	C	120	ILE	2.5
1	A	123	LYS	2.4
1	B	202	LYS	2.4
1	D	28	TYR	2.4
1	C	118	LEU	2.4
1	B	215	SER	2.4
1	C	113	LEU	2.3
1	D	111	THR	2.3
1	A	26	ARG	2.3
1	D	120	ILE	2.3
1	C	134	PRO	2.3
1	C	124	ASP	2.3
1	D	109	ILE	2.3
1	C	217	GLY	2.2
1	C	122	LYS	2.2
1	C	107	GLU	2.0
1	C	203	MET	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($Å^2$)	Q<0.9
1	RPI	D	16	15/16	0.79	0.21	36,54,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	RPI	C	16	15/16	0.80	0.20	35,70,99,113	0
1	RPI	A	16	15/16	0.80	0.22	19,53,75,79	0
1	RPI	B	16	15/16	0.81	0.22	26,45,76,90	0

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(Å²)	Q<0.9
3	3PG	D	301	11/11	0.62	0.21	52,56,71,82	0
4	PG4	A	303	13/13	0.71	0.22	43,53,62,67	0
4	PG4	C	301	7/13	0.72	0.21	50,56,68,70	0
4	PG4	B	304	7/13	0.75	0.18	47,57,64,67	0
4	PG4	B	302	7/13	0.76	0.17	35,44,52,53	0
4	PG4	A	304	6/13	0.77	0.18	44,53,57,59	0
4	PG4	C	302	7/13	0.78	0.22	59,68,74,75	0
4	PG4	D	302	7/13	0.78	0.18	45,49,57,58	0
5	SO4	B	307	5/5	0.78	0.10	63,72,76,87	0
5	SO4	C	303	5/5	0.81	0.13	46,57,70,71	0
3	3PG	A	302	11/11	0.84	0.16	38,44,58,63	0
4	PG4	B	305	9/13	0.86	0.15	33,49,57,63	0
3	3PG	B	301	11/11	0.86	0.16	36,45,58,65	0
5	SO4	B	306	5/5	0.88	0.10	64,65,75,77	0
5	SO4	D	304	5/5	0.88	0.18	47,55,60,65	0
5	SO4	D	303	5/5	0.89	0.11	63,65,74,75	0
4	PG4	B	303	7/13	0.90	0.11	37,44,47,50	0
4	PG4	A	305	10/13	0.91	0.11	38,44,52,52	0
2	CL	A	301	1/1	0.94	0.11	56,56,56,56	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.
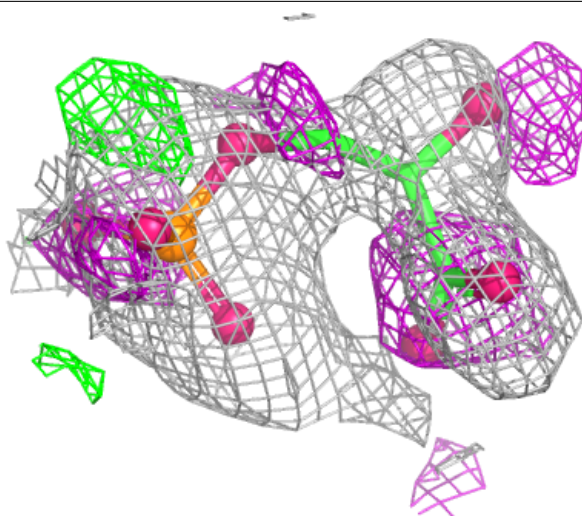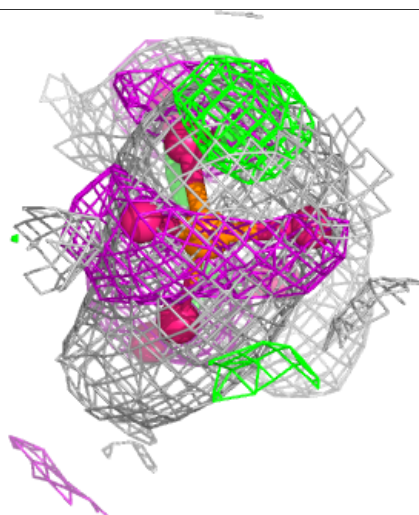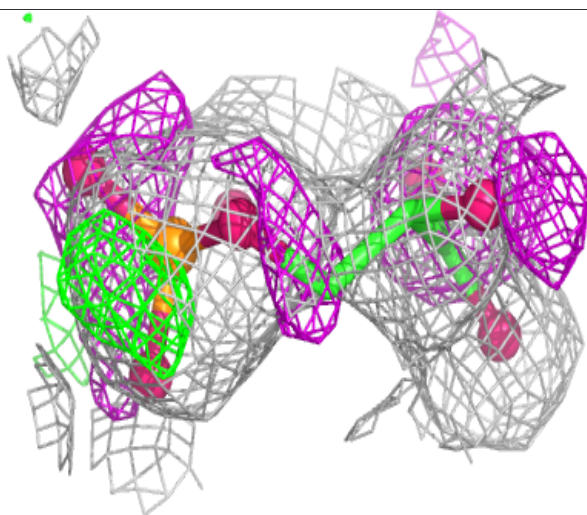
Electron density around 3PG D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
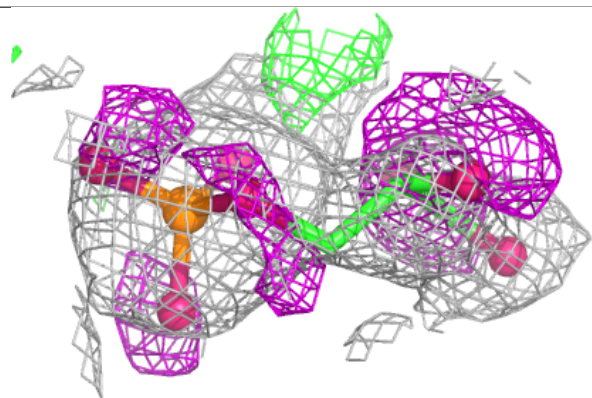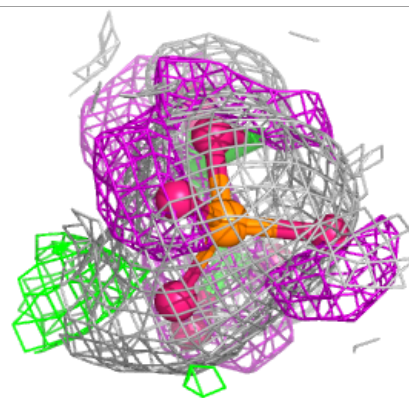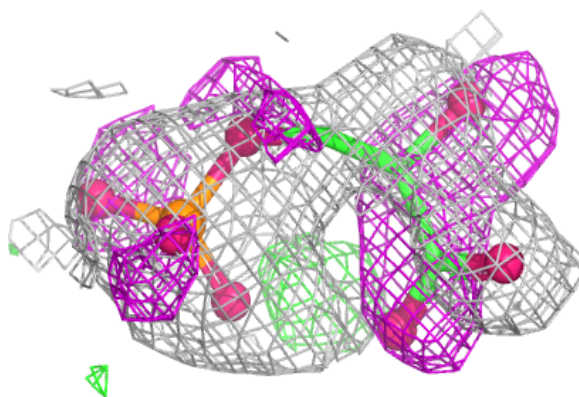and green (positive)
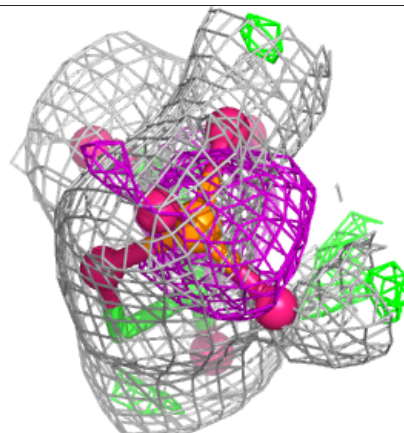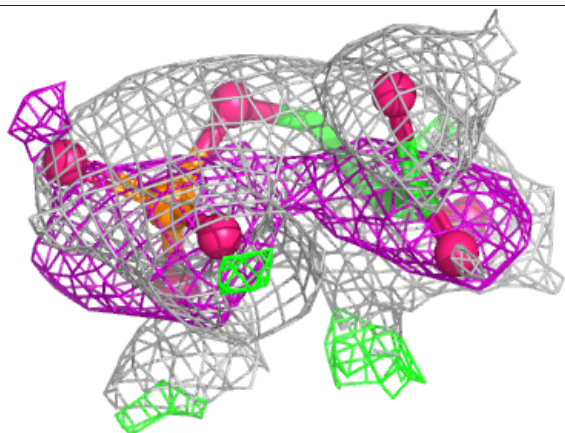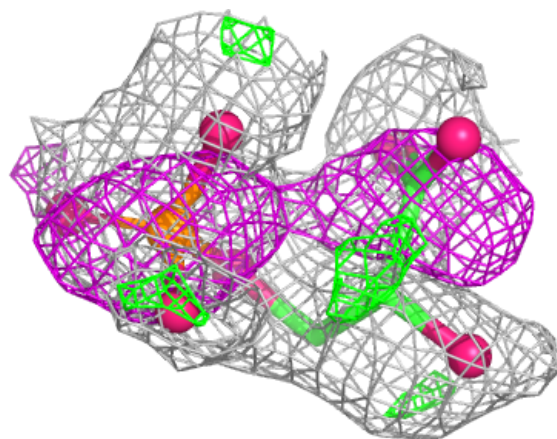
Electron density around 3PG A 302:

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

Electron density around 3PG B 301:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.