



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:03 PM UTC

PDB ID : 1VKJ / pdb_00001vkj
Title : Crystal structure of heparan sulfate 3-O-sulfotransferase isoform 1 in the presence of PAP
Authors : Thorp, S.; Lee, K.A.; Negishi, M.; Linhardt, R.J.; Liu, J.; Pedersen, L.C.
Deposited on : 2004-05-25
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

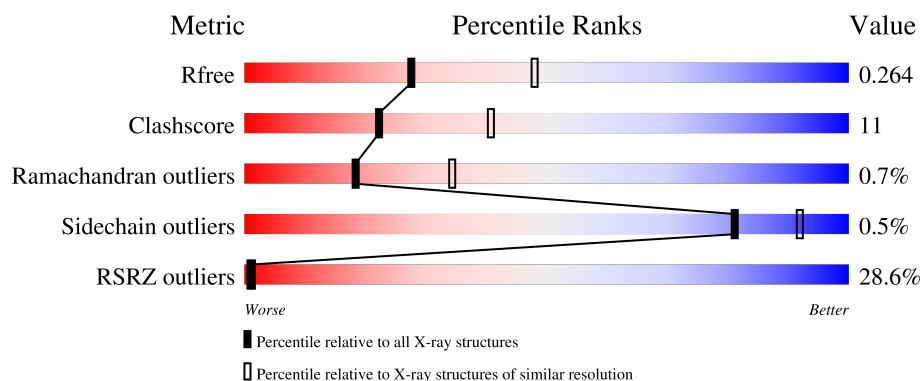
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	285	5% 71% 19% • 9%
1	B	285	3% 72% 18% 9%
1	C	285	69% 60% 25% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6265 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 heparan sulfate (glucosamine) 3-O-sulfotransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2113	1366	374	366	7			
1	B	258	Total	C	N	O	S	0	0	0
			2126	1375	378	366	7			
1	C	247	Total	C	N	O	S	0	0	0
			1757	1133	306	314	4			

There are 63 discrepancies between the modelled and reference sequences:

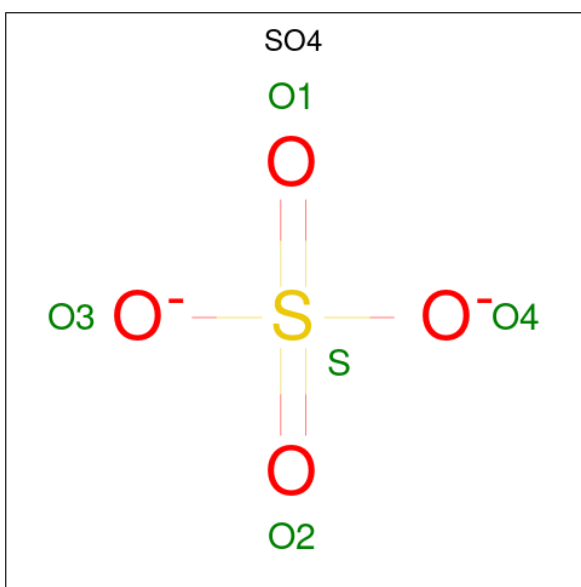
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP O35310
A	28	GLY	-	expression tag	UNP O35310
A	29	SER	-	expression tag	UNP O35310
A	30	SER	-	expression tag	UNP O35310
A	31	HIS	-	expression tag	UNP O35310
A	32	HIS	-	expression tag	UNP O35310
A	33	HIS	-	expression tag	UNP O35310
A	34	HIS	-	expression tag	UNP O35310
A	35	HIS	-	expression tag	UNP O35310
A	36	HIS	-	expression tag	UNP O35310
A	37	SER	-	expression tag	UNP O35310
A	38	SER	-	expression tag	UNP O35310
A	39	GLY	-	expression tag	UNP O35310
A	40	LEU	-	expression tag	UNP O35310
A	41	VAL	-	expression tag	UNP O35310
A	42	PRO	-	expression tag	UNP O35310
A	43	ARG	-	expression tag	UNP O35310
A	44	GLY	-	expression tag	UNP O35310
A	45	SER	-	expression tag	UNP O35310
A	46	HIS	-	expression tag	UNP O35310
A	47	MET	-	expression tag	UNP O35310
B	27	MET	-	expression tag	UNP O35310
B	28	GLY	-	expression tag	UNP O35310

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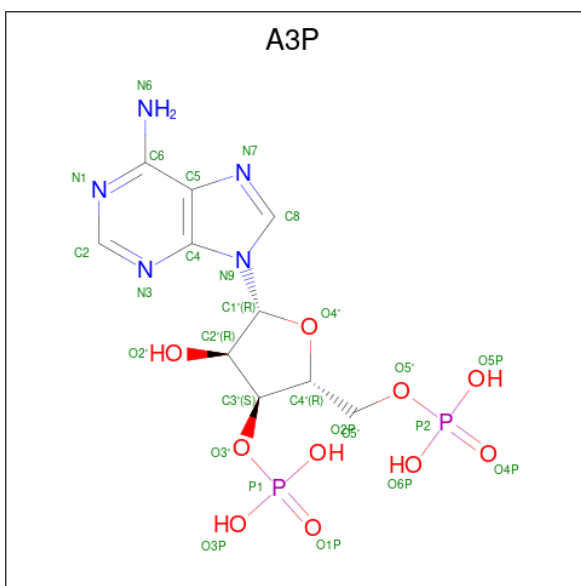
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP O35310
B	30	SER	-	expression tag	UNP O35310
B	31	HIS	-	expression tag	UNP O35310
B	32	HIS	-	expression tag	UNP O35310
B	33	HIS	-	expression tag	UNP O35310
B	34	HIS	-	expression tag	UNP O35310
B	35	HIS	-	expression tag	UNP O35310
B	36	HIS	-	expression tag	UNP O35310
B	37	SER	-	expression tag	UNP O35310
B	38	SER	-	expression tag	UNP O35310
B	39	GLY	-	expression tag	UNP O35310
B	40	LEU	-	expression tag	UNP O35310
B	41	VAL	-	expression tag	UNP O35310
B	42	PRO	-	expression tag	UNP O35310
B	43	ARG	-	expression tag	UNP O35310
B	44	GLY	-	expression tag	UNP O35310
B	45	SER	-	expression tag	UNP O35310
B	46	HIS	-	expression tag	UNP O35310
B	47	MET	-	expression tag	UNP O35310
C	27	MET	-	expression tag	UNP O35310
C	28	GLY	-	expression tag	UNP O35310
C	29	SER	-	expression tag	UNP O35310
C	30	SER	-	expression tag	UNP O35310
C	31	HIS	-	expression tag	UNP O35310
C	32	HIS	-	expression tag	UNP O35310
C	33	HIS	-	expression tag	UNP O35310
C	34	HIS	-	expression tag	UNP O35310
C	35	HIS	-	expression tag	UNP O35310
C	36	HIS	-	expression tag	UNP O35310
C	37	SER	-	expression tag	UNP O35310
C	38	SER	-	expression tag	UNP O35310
C	39	GLY	-	expression tag	UNP O35310
C	40	LEU	-	expression tag	UNP O35310
C	41	VAL	-	expression tag	UNP O35310
C	42	PRO	-	expression tag	UNP O35310
C	43	ARG	-	expression tag	UNP O35310
C	44	GLY	-	expression tag	UNP O35310
C	45	SER	-	expression tag	UNP O35310
C	46	HIS	-	expression tag	UNP O35310
C	47	MET	-	expression tag	UNP O35310

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

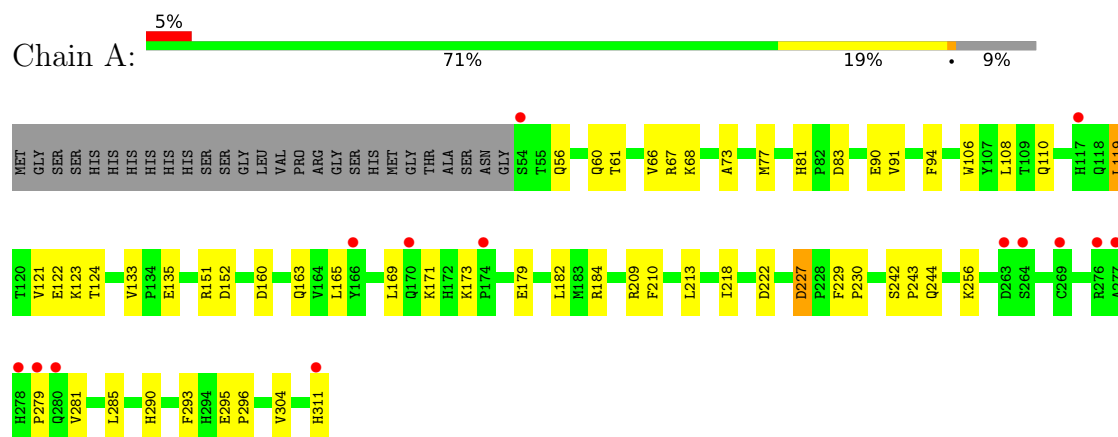
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	98	Total	O	0	0
			98	98		
4	C	1	Total	O	0	0
			1	1		

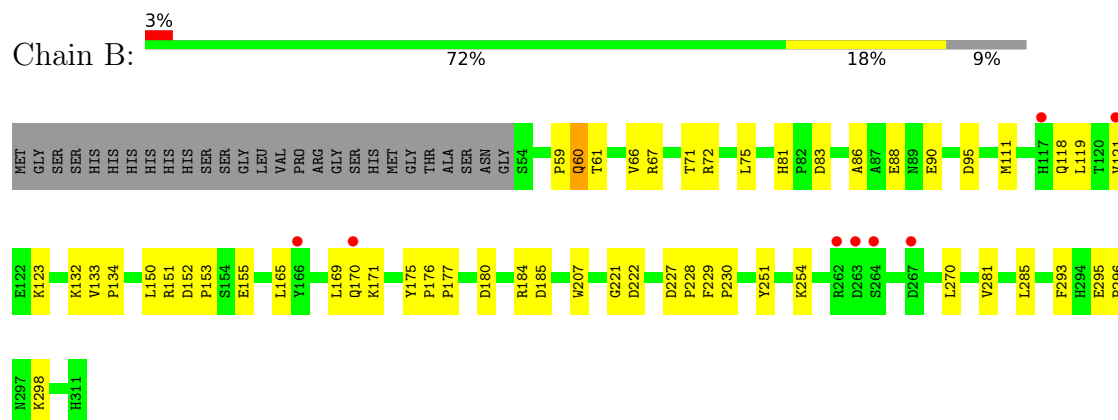
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

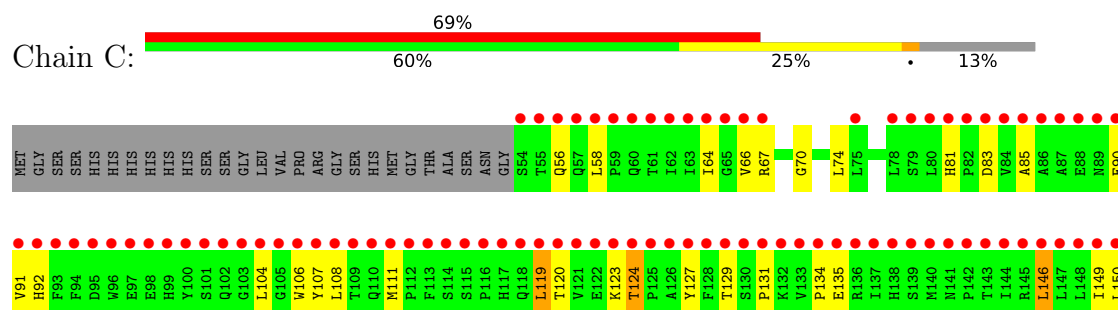
- Molecule 1: heparan sulfate (glucosamine) 3-O-sulfotransferase 1

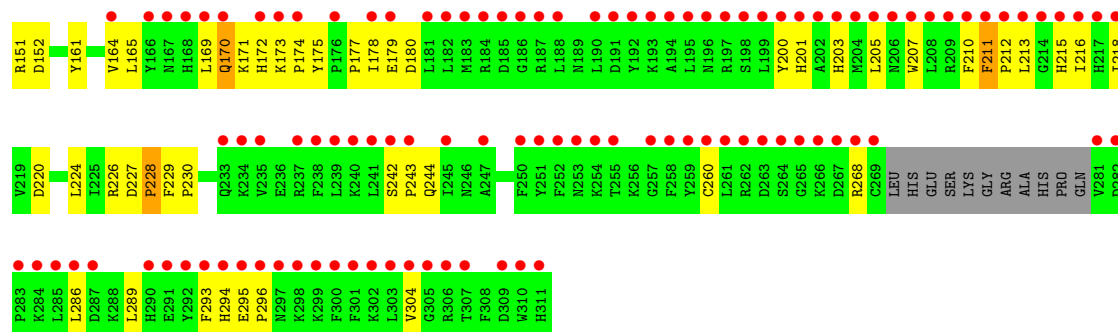


- Molecule 1: heparan sulfate (glucosamine) 3-O-sulfotransferase 1



- Molecule 1: heparan sulfate (glucosamine) 3-O-sulfotransferase 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	300.14Å 300.14Å 84.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.50 24.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.6 (24.84-2.50) 90.6 (24.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.264 0.243 , 0.264	Depositor DCC
R_{free} test set	3225 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A3P, SO4

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	0.50	0/2179	0.93	6/2959 (0.2%)
1	B	0.49	0/2193	0.94	6/2975 (0.2%)
1	C	0.69	0/1809	1.09	14/2488 (0.6%)
All	All	0.56	0/6181	0.98	26/8422 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	THR	CA-C-N	7.47	128.14	119.47
1	C	124	THR	C-N-CA	7.47	128.14	119.47
1	A	133	VAL	N-CA-C	7.35	121.17	112.35
1	A	227	ASP	CA-C-N	7.02	128.61	119.84
1	A	227	ASP	C-N-CA	7.02	128.61	119.84
1	C	64	ILE	N-CA-C	6.64	119.40	112.83
1	B	227	ASP	CA-C-N	6.55	128.03	119.84
1	B	227	ASP	C-N-CA	6.55	128.03	119.84
1	C	146	LEU	N-CA-C	6.38	119.86	109.59
1	B	60	GLN	N-CA-C	-5.94	106.03	113.28
1	C	106	TRP	N-CA-C	-5.87	104.80	111.14
1	A	60	GLN	N-CA-C	-5.73	106.13	113.23
1	B	118	GLN	N-CA-C	5.69	118.94	110.52
1	B	95	ASP	N-CA-C	5.49	119.98	113.28
1	C	58	LEU	CA-C-N	5.48	126.69	119.84
1	C	58	LEU	C-N-CA	5.48	126.69	119.84
1	C	174	PRO	N-CA-C	5.47	120.68	111.32
1	A	94	PHE	N-CA-C	5.45	117.98	111.71
1	C	218	ILE	N-CA-C	5.40	115.41	107.15
1	C	170	GLN	N-CA-C	-5.36	106.59	113.02
1	B	133	VAL	N-CA-C	5.23	120.17	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	ASP	CA-C-N	5.21	126.36	119.84
1	C	227	ASP	C-N-CA	5.21	126.36	119.84
1	C	211	PHE	CA-C-N	5.11	125.91	120.13
1	C	211	PHE	C-N-CA	5.11	125.91	120.13
1	A	182	LEU	N-CA-C	5.11	116.93	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2113	0	2054	39	0
1	B	2126	0	2081	34	0
1	C	1757	0	1470	53	1
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	81	0	33	2	0
4	A	79	0	0	3	0
4	B	98	0	0	3	0
4	C	1	0	0	0	0
All	All	6265	0	5638	124	1

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 11.

All (124) 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:60:GLN:HB2	1:B:119:LEU:CD1	2.14	0.77
1:A:218:ILE:HD12	1:A:304:VAL:HG11	1.66	0.75
1:C:119:LEU:C	1:C:119:LEU:HD12	2.18	0.68
1:A:279:PRO:O	1:A:281:VAL:HG23	1.93	0.68
1:B:254:LYS:HB2	1:C:230:PRO:HG3	1.74	0.68
1:B:61:THR:HG23	1:B:121:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:HIS:CE1	1:C:205:LEU:HD11	2.31	0.66
1:B:60:GLN:HB2	1:B:119:LEU:HD13	1.77	0.65
1:A:61:THR:HG23	1:A:121:VAL:HG13	1.76	0.65
1:B:177:PRO:HD2	1:B:180:ASP:OD2	1.96	0.65
1:A:119:LEU:C	1:A:119:LEU:HD12	2.21	0.65
1:C:129:THR:HG22	1:C:203:HIS:CE1	2.32	0.65
1:A:119:LEU:HD12	1:A:119:LEU:O	1.97	0.65
1:B:151:ARG:HB2	1:B:222:ASP:OD1	1.97	0.64
1:C:66:VAL:HG22	1:C:67:ARG:N	2.12	0.64
1:C:66:VAL:HG22	1:C:67:ARG:H	1.64	0.62
1:A:151:ARG:HB2	1:A:222:ASP:OD1	2.01	0.60
1:B:295:GLU:OE2	1:B:298:LYS:HE2	2.00	0.60
1:B:229:PHE:HB3	1:B:230:PRO:HD3	1.82	0.60
1:C:150:LEU:HD13	1:C:200:TYR:CD1	2.37	0.60
1:A:295:GLU:HB3	1:A:296:PRO:HD3	1.84	0.59
1:C:74:LEU:HD12	1:C:74:LEU:O	2.01	0.59
1:C:81:HIS:CE1	1:C:83:ASP:HB2	2.39	0.58
1:A:229:PHE:HB3	1:A:230:PRO:HD3	1.83	0.58
1:C:293:PHE:C	1:C:296:PRO:HD2	2.28	0.58
1:A:165:LEU:O	1:A:169:LEU:HD12	2.04	0.58
1:C:119:LEU:HD12	1:C:119:LEU:O	2.06	0.56
1:C:151:ARG:O	1:C:152:ASP:C	2.49	0.56
1:A:122:GLU:OE2	1:A:124:THR:OG1	2.24	0.56
1:C:149:ILE:O	1:C:149:ILE:HG23	2.06	0.55
1:B:71:THR:HB	1:B:123:LYS:HD2	1.88	0.55
1:B:90:GLU:HA	1:B:123:LYS:O	2.06	0.55
1:C:229:PHE:HB3	1:C:230:PRO:HD3	1.89	0.55
1:C:201:HIS:HE1	1:C:205:LEU:HD11	1.71	0.55
1:A:281:VAL:HG13	1:A:285:LEU:HD23	1.89	0.54
1:B:59:PRO:HG3	1:B:111:MET:SD	2.47	0.54
1:B:151:ARG:HA	4:B:619:HOH:O	2.08	0.53
1:C:212:PRO:O	1:C:213:LEU:C	2.48	0.53
1:B:228:PRO:HD2	4:B:633:HOH:O	2.09	0.52
1:A:281:VAL:CG1	1:A:285:LEU:HD23	2.40	0.52
1:B:165:LEU:O	1:B:169:LEU:HD13	2.11	0.51
1:C:165:LEU:O	1:C:169:LEU:HD12	2.11	0.50
1:B:293:PHE:C	1:B:296:PRO:HD2	2.36	0.50
1:C:161:TYR:CG	1:C:178:ILE:HD13	2.47	0.50
1:C:131:PRO:O	1:C:134:PRO:HD2	2.12	0.50
1:A:67:ARG:HG2	1:A:68:LYS:HG2	1.94	0.49
1:C:90:GLU:HA	1:C:123:LYS:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ASP:HB3	1:B:155:GLU:CG	2.42	0.49
1:A:66:VAL:HG22	1:A:67:ARG:N	2.28	0.49
1:B:169:LEU:C	1:B:171:LYS:H	2.20	0.49
1:C:124:THR:HG21	1:C:127:TYR:CE2	2.47	0.49
1:B:72:ARG:HD3	2:B:602:SO4:O1	2.13	0.49
1:C:171:LYS:O	1:C:173:LYS:N	2.45	0.49
1:A:91:VAL:HG21	1:A:122:GLU:HG3	1.94	0.48
1:B:281:VAL:HG13	1:B:285:LEU:HD23	1.95	0.48
1:A:290:HIS:CE1	1:A:311:HIS:CD2	3.02	0.48
1:C:107:TYR:O	1:C:111:MET:HE3	2.13	0.48
1:A:218:ILE:CD1	1:A:304:VAL:HG11	2.40	0.47
1:A:304:VAL:O	1:A:304:VAL:HG12	2.14	0.47
1:A:227:ASP:O	1:A:230:PRO:HD2	2.14	0.47
1:B:81:HIS:CE1	1:B:83:ASP:HB2	2.49	0.47
1:A:293:PHE:C	1:A:296:PRO:HD2	2.40	0.47
1:B:75:LEU:HD11	1:B:86:ALA:HB1	1.97	0.47
1:C:293:PHE:O	1:C:296:PRO:HD2	2.14	0.47
1:A:209:ARG:HG2	1:A:210:PHE:CE2	2.50	0.46
1:A:90:GLU:HA	1:A:123:LYS:O	2.14	0.46
1:C:242:SER:O	1:C:244:GLN:N	2.49	0.46
1:B:66:VAL:HG22	1:B:67:ARG:N	2.30	0.46
1:A:242:SER:O	1:A:244:GLN:N	2.49	0.46
1:C:260:CYS:HB3	1:C:268:ARG:O	2.16	0.45
1:C:91:VAL:O	1:C:92:HIS:HB2	2.17	0.45
1:C:146:LEU:O	1:C:216:ILE:HA	2.17	0.45
1:C:165:LEU:HG	1:C:169:LEU:CD1	2.47	0.45
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.83	0.44
1:C:224:LEU:O	1:C:228:PRO:HG3	2.18	0.44
1:B:71:THR:CB	1:B:123:LYS:HD2	2.47	0.44
1:C:124:THR:HB	1:C:127:TYR:CZ	2.53	0.44
1:C:228:PRO:O	1:C:229:PHE:C	2.61	0.44
1:A:81:HIS:CE1	1:A:83:ASP:HB2	2.53	0.43
1:A:213:LEU:HD11	1:A:304:VAL:HG13	1.99	0.43
1:B:184:ARG:HG2	1:B:185:ASP:OD2	2.18	0.43
1:C:56:GLN:C	1:C:108:LEU:HD11	2.44	0.43
1:C:85:ALA:O	1:C:120:THR:HA	2.18	0.43
1:B:251:TYR:CZ	1:C:226:ARG:HD2	2.53	0.43
1:C:295:GLU:CB	1:C:296:PRO:HD3	2.48	0.43
1:A:160:ASP:O	1:A:163:GLN:HB3	2.17	0.43
1:B:88:GLU:OE1	1:B:88:GLU:HA	2.19	0.43
1:C:119:LEU:C	1:C:119:LEU:CD1	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:HIS:O	1:C:207:TRP:HD1	2.01	0.43
1:A:151:ARG:O	1:A:152:ASP:C	2.59	0.43
1:A:179:GLU:HB3	4:A:644:HOH:O	2.18	0.43
3:A:604:A3P:O4'	1:C:70:GLY:HA2	2.19	0.43
1:B:90:GLU:HG2	1:B:123:LYS:O	2.19	0.43
1:A:151:ARG:HA	4:A:628:HOH:O	2.19	0.43
3:A:603:A3P:C2	1:B:270:LEU:HD12	2.49	0.43
1:C:66:VAL:CG2	1:C:67:ARG:N	2.81	0.43
1:C:220:ASP:OD1	1:C:220:ASP:C	2.62	0.42
1:A:256:LYS:HE2	4:A:631:HOH:O	2.18	0.42
1:C:286:LEU:O	1:C:289:LEU:HB2	2.19	0.42
1:C:161:TYR:CD2	1:C:161:TYR:C	2.97	0.42
1:C:213:LEU:HD21	1:C:304:VAL:O	2.19	0.42
1:C:164:VAL:HG11	1:C:175:TYR:CZ	2.55	0.42
1:B:152:ASP:HB3	1:B:155:GLU:HG3	2.01	0.42
1:B:134:PRO:HG3	1:B:207:TRP:CE2	2.54	0.41
1:C:170:GLN:HA	1:C:170:GLN:OE1	2.19	0.41
1:A:209:ARG:HG2	1:A:210:PHE:CD2	2.55	0.41
1:C:171:LYS:C	1:C:173:LYS:N	2.76	0.41
1:C:211:PHE:HA	1:C:212:PRO:HD3	1.78	0.41
1:A:165:LEU:O	1:A:169:LEU:CD1	2.68	0.41
1:C:135:GLU:CB	1:C:210:PHE:CZ	3.04	0.41
1:A:169:LEU:C	1:A:171:LYS:H	2.29	0.41
1:C:177:PRO:O	1:C:180:ASP:HB2	2.21	0.41
1:A:73:ALA:O	1:A:77:MET:HG3	2.21	0.41
1:A:171:LYS:C	1:A:173:LYS:H	2.29	0.41
1:B:150:LEU:O	1:B:221:GLY:N	2.52	0.41
1:C:293:PHE:O	1:C:294:HIS:C	2.63	0.41
1:A:135:GLU:HB2	1:A:210:PHE:CZ	2.56	0.41
1:A:56:GLN:O	1:A:108:LEU:HD11	2.21	0.41
1:B:152:ASP:HA	1:B:153:PRO:HD3	1.97	0.41
1:A:106:TRP:O	1:A:110:GLN:HG2	2.21	0.40
1:C:108:LEU:O	1:C:108:LEU:HG	2.19	0.40
1:B:132:LYS:HG2	4:B:613:HOH:O	2.21	0.40
1:B:175:TYR:HA	1:B:176:PRO:HD3	1.88	0.40
1:C:178:ILE:HG23	1:C:179:GLU:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LEU:CD1	1:C:104:LEU:CD1[7_455]	1.74	0.46

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/285 (90%)	239 (93%)	16 (6%)	1 (0%)	30	49
1	B	256/285 (90%)	246 (96%)	9 (4%)	1 (0%)	30	49
1	C	243/285 (85%)	214 (88%)	26 (11%)	3 (1%)	10	20
All	All	755/855 (88%)	699 (93%)	51 (7%)	5 (1%)	18	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	HIS
1	C	228	PRO
1	B	170	GLN
1	C	243	PRO
1	A	243	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/258 (88%)	225 (100%)	1 (0%)	84	93
1	B	229/258 (89%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	148/258 (57%)	146 (99%)	2 (1%)	59	81
All	All	603/774 (78%)	600 (100%)	3 (0%)	81	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	C	119	LEU
1	C	215	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	290	HIS
1	A	311	HIS
1	B	170	GLN
1	B	271	HIS
1	C	311	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
2	SO4	A	601	-	4,4,4	0.38	0	6,6,6	0.06	0
3	A3P	A	603	-	29,29,29	0.55	0	44,45,45	0.82	1 (2%)
2	SO4	B	602	-	4,4,4	0.40	0	6,6,6	0.08	0
3	A3P	A	602	-	29,29,29	0.57	0	44,45,45	0.65	0
3	A3P	A	604	-	29,29,29	0.36	0	44,45,45	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A3P	A	602	-	-	5/15/31/31	0/3/3/3
3	A3P	A	604	-	-	4/15/31/31	0/3/3/3
3	A3P	A	603	-	-	1/15/31/31	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	A3P	O5'-P2-O4P	-2.14	100.66	106.44

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	A3P	C2'-C1'-N9-C8
3	A	602	A3P	C2'-C1'-N9-C4
3	A	604	A3P	C3'-O3'-P1-O1P
3	A	602	A3P	O4'-C1'-N9-C8
3	A	604	A3P	O4'-C1'-N9-C8
3	A	602	A3P	C4'-C3'-O3'-P1
3	A	604	A3P	C2'-C1'-N9-C8
3	A	604	A3P	C3'-C4'-C5'-O5'
3	A	603	A3P	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	A	602	A3P	C2'-C3'-O3'-P1

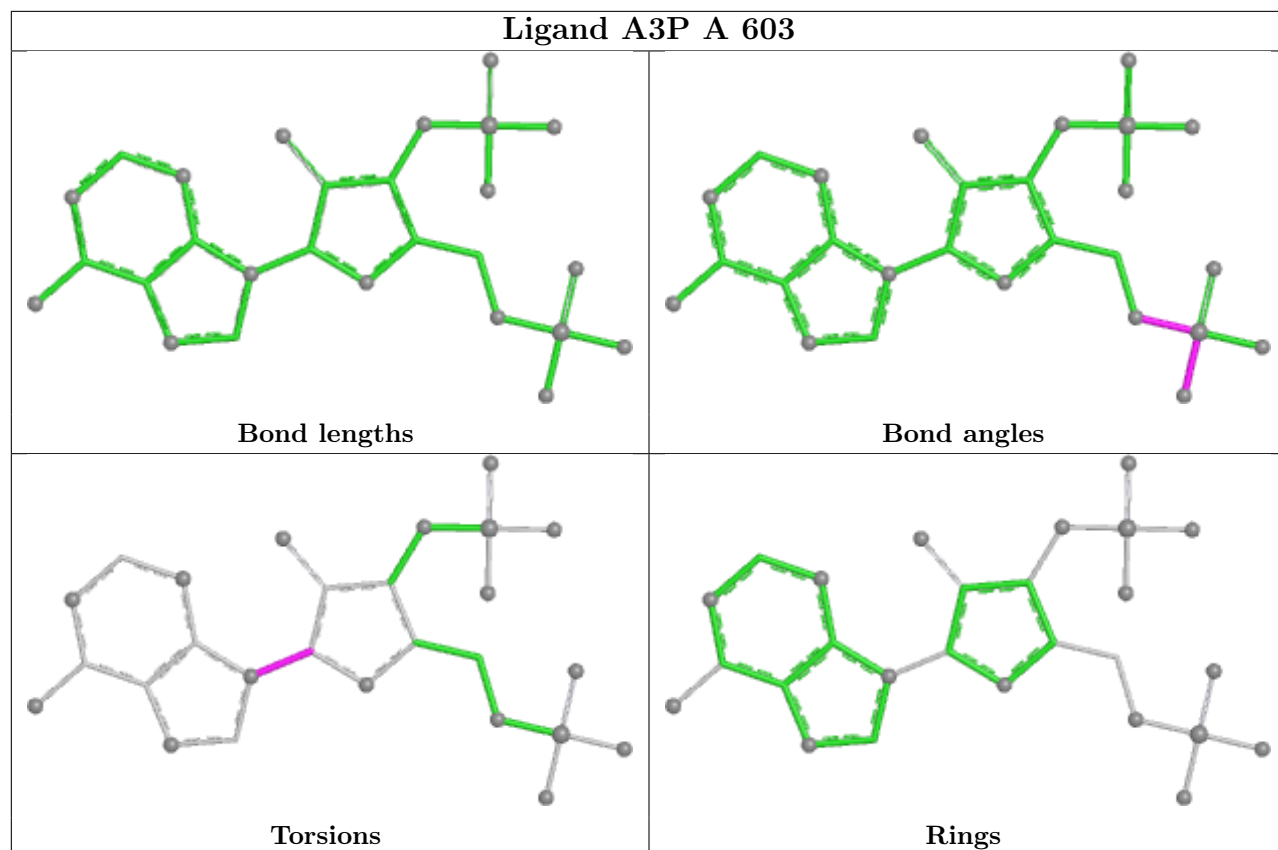
There are no ring outliers.

3 monomers are involved in 3 short contacts:

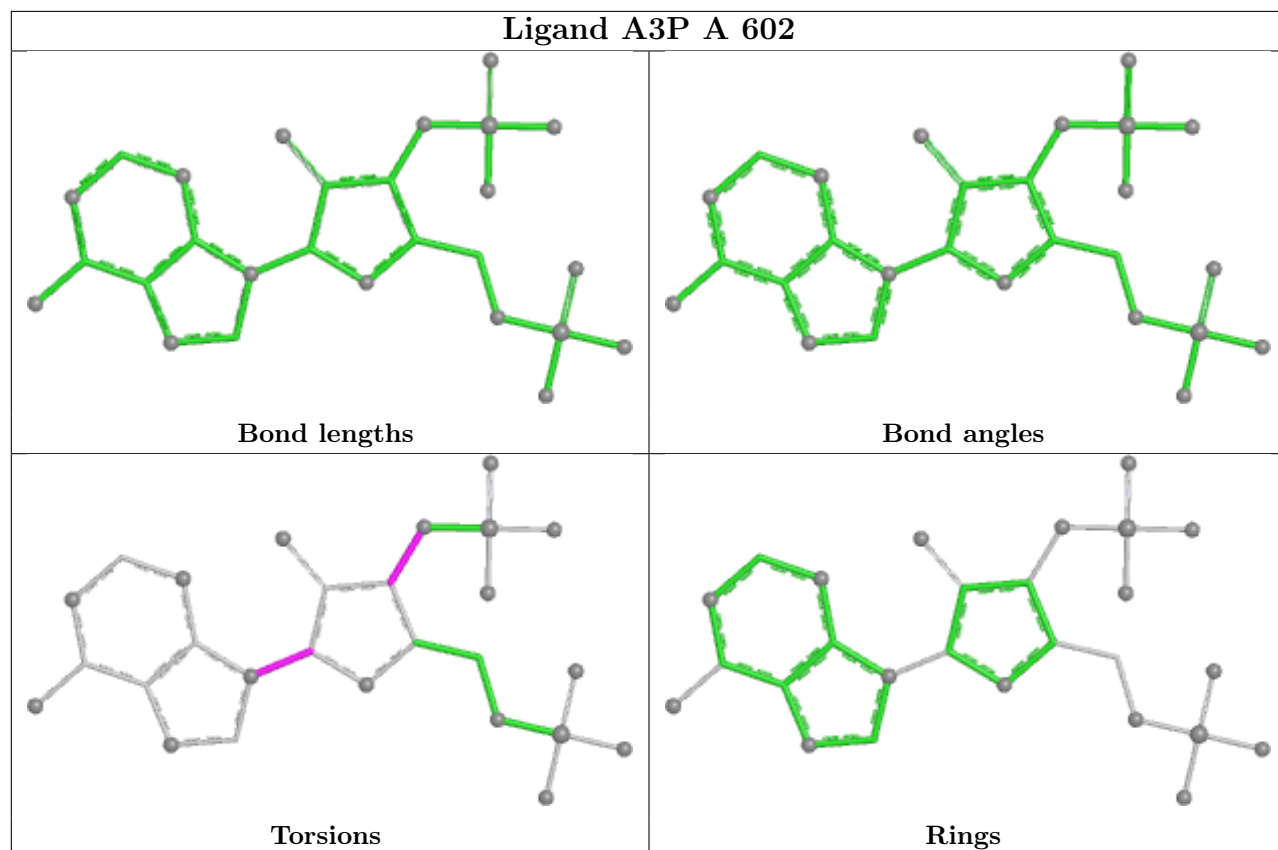
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	A3P	1	0
2	B	602	SO4	1	0
3	A	604	A3P	1	0

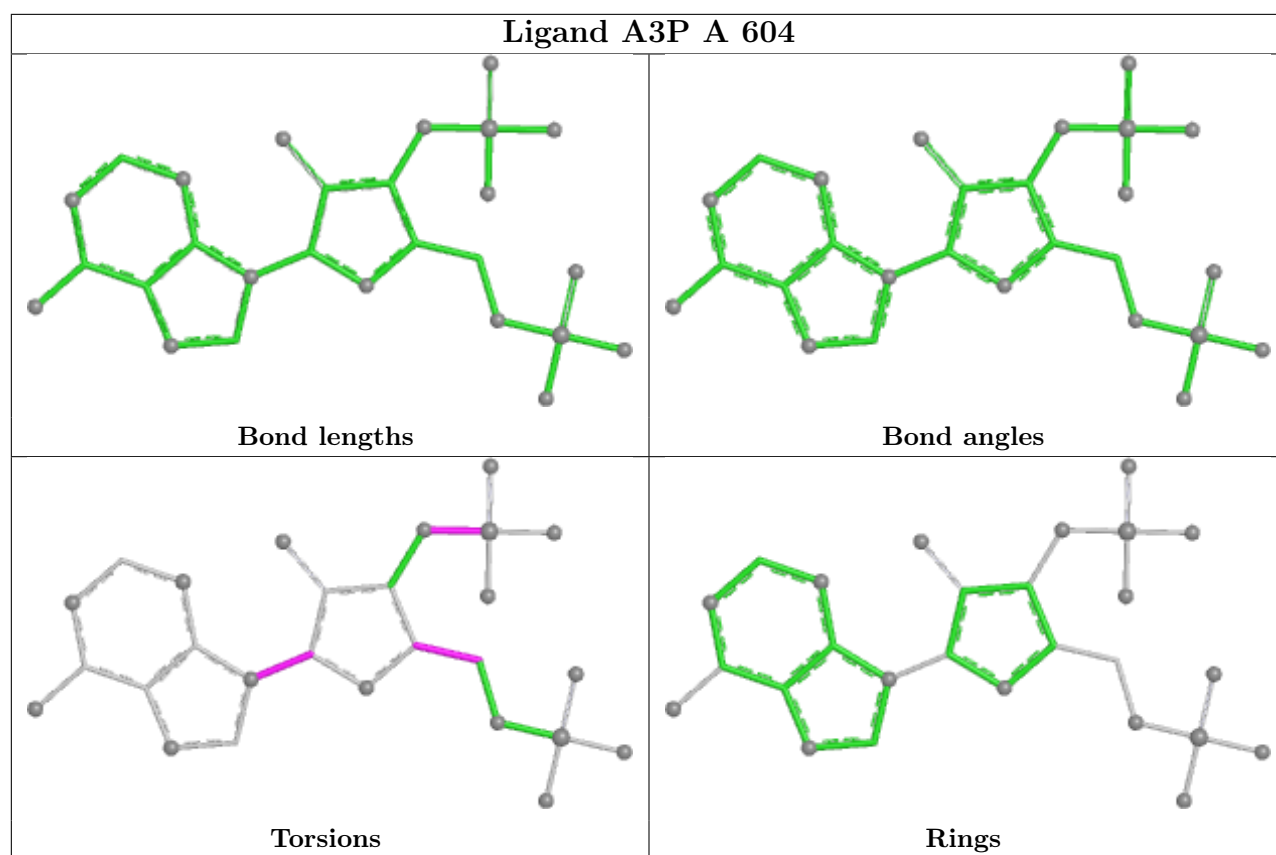
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand A3P A 603



Ligand A3P A 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/285 (90%)	0.18	14 (5%) 31 27	24, 41, 70, 90	0
1	B	258/285 (90%)	-0.08	8 (3%) 51 47	22, 37, 63, 78	0
1	C	247/285 (86%)	3.63	196 (79%) 0 0	52, 106, 129, 135	0
All	All	763/855 (89%)	1.21	218 (28%) 1 1	22, 47, 124, 135	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	TYR	11.2
1	C	94	PHE	8.6
1	C	133	VAL	8.5
1	C	144	ILE	8.3
1	C	101	SER	8.1
1	C	107	TYR	8.1
1	C	57	GLN	7.8
1	C	145	ARG	7.5
1	C	61	THR	7.4
1	C	93	PHE	7.4
1	C	137	ILE	7.3
1	C	139	SER	7.2
1	C	263	ASP	7.1
1	C	55	THR	7.0
1	C	62	ILE	7.0
1	C	96	TRP	7.0
1	C	211	PHE	6.9
1	C	140	MET	6.9
1	C	113	PHE	6.8
1	C	185	ASP	6.8
1	C	110	GLN	6.6
1	C	132	LYS	6.6
1	C	104	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	143	THR	6.5
1	C	146	LEU	6.5
1	C	114	SER	6.5
1	C	210	PHE	6.5
1	C	138	HIS	6.4
1	C	60	GLN	6.3
1	C	281	VAL	6.3
1	C	186	GLY	6.3
1	C	216	ILE	6.3
1	C	59	PRO	6.2
1	C	212	PRO	6.2
1	C	269	CYS	6.2
1	C	214	GLY	6.1
1	C	58	LEU	6.0
1	C	117	HIS	5.9
1	C	131	PRO	5.9
1	C	136	ARG	5.7
1	C	239	LEU	5.7
1	C	95	ASP	5.7
1	C	56	GLN	5.7
1	C	92	HIS	5.6
1	C	121	VAL	5.6
1	C	172	HIS	5.6
1	C	98	GLU	5.6
1	C	264	SER	5.5
1	C	206	ASN	5.5
1	C	266	LYS	5.4
1	C	294	HIS	5.4
1	C	120	THR	5.4
1	A	278	HIS	5.3
1	C	102	GLN	5.2
1	C	122	GLU	5.2
1	C	142	PRO	5.2
1	C	213	LEU	5.2
1	C	85	ALA	5.1
1	C	303	LEU	5.1
1	C	215	HIS	5.0
1	C	282	ASP	5.0
1	C	245	ILE	4.9
1	C	119	LEU	4.9
1	C	208	LEU	4.9
1	C	207	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	127	TYR	4.9
1	C	99	HIS	4.8
1	C	304	VAL	4.8
1	C	209	ARG	4.8
1	C	200	TYR	4.8
1	C	89	ASN	4.8
1	C	103	GLY	4.8
1	C	112	PRO	4.7
1	C	54	SER	4.7
1	C	116	PRO	4.6
1	C	134	PRO	4.6
1	C	86	ALA	4.5
1	C	201	HIS	4.5
1	C	260	CYS	4.5
1	C	184	ARG	4.4
1	C	268	ARG	4.4
1	C	251	TYR	4.4
1	C	115	SER	4.4
1	C	91	VAL	4.4
1	C	238	PHE	4.3
1	C	147	LEU	4.3
1	B	170	GLN	4.3
1	C	295	GLU	4.3
1	C	286	LEU	4.3
1	A	264	SER	4.2
1	C	105	GLY	4.2
1	C	262	ARG	4.2
1	C	88	GLU	4.2
1	C	106	TRP	4.2
1	C	204	MET	4.2
1	C	130	SER	4.1
1	C	203	HIS	4.0
1	C	241	LEU	4.0
1	C	183	MET	4.0
1	C	118	GLN	4.0
1	C	64	ILE	4.0
1	C	170	GLN	3.9
1	C	217	HIS	3.9
1	C	187	ARG	3.9
1	C	65	GLY	3.9
1	C	284	LYS	3.8
1	C	235	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	202	ALA	3.8
1	C	141	ASN	3.8
1	C	247	ALA	3.7
1	C	188	LEU	3.7
1	C	243	PRO	3.7
1	C	135	GLU	3.7
1	C	108	LEU	3.7
1	C	79	SER	3.6
1	C	298	LYS	3.6
1	C	148	LEU	3.6
1	C	261	LEU	3.6
1	C	301	PHE	3.5
1	C	307	THR	3.5
1	C	300	PHE	3.5
1	C	63	ILE	3.4
1	C	195	LEU	3.4
1	C	199	LEU	3.4
1	C	97	GLU	3.4
1	C	84	VAL	3.3
1	B	264	SER	3.3
1	C	128	PHE	3.3
1	B	166	TYR	3.3
1	C	191	ASP	3.3
1	C	125	PRO	3.3
1	C	124	THR	3.3
1	C	293	PHE	3.2
1	C	292	TYR	3.2
1	B	117	HIS	3.2
1	C	166	TYR	3.2
1	C	267	ASP	3.2
1	C	82	PRO	3.2
1	C	90	GLU	3.2
1	C	126	ALA	3.1
1	A	170	GLN	3.1
1	C	190	LEU	3.1
1	C	181	LEU	3.1
1	C	205	LEU	3.1
1	C	87	ALA	3.1
1	A	279	PRO	3.1
1	C	173	LYS	3.0
1	C	109	THR	3.0
1	A	263	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	179	GLU	2.9
1	C	150	LEU	2.9
1	C	259	TYR	2.9
1	C	258	PHE	2.9
1	C	265	GLY	2.9
1	C	111	MET	2.9
1	C	311	HIS	2.9
1	C	287	ASP	2.9
1	C	306	ARG	2.9
1	C	302	LYS	2.9
1	C	250	PHE	2.9
1	C	252	PHE	2.9
1	C	66	VAL	2.9
1	C	169	LEU	2.9
1	C	257	GLY	2.9
1	C	218	ILE	2.8
1	B	263	ASP	2.8
1	C	129	THR	2.8
1	C	299	LYS	2.8
1	A	54	SER	2.8
1	C	291	GLU	2.8
1	C	192	TYR	2.7
1	C	123	LYS	2.7
1	C	254	LYS	2.7
1	C	75	LEU	2.7
1	C	78	LEU	2.7
1	C	283	PRO	2.7
1	C	305	GLY	2.6
1	A	280	GLN	2.6
1	C	255	THR	2.6
1	A	166	TYR	2.5
1	A	174	PRO	2.5
1	A	276	ARG	2.5
1	C	178	ILE	2.5
1	C	233	GLN	2.5
1	C	253	ASN	2.5
1	C	285	LEU	2.5
1	C	297	ASN	2.5
1	C	237	ARG	2.4
1	C	83	ASP	2.4
1	C	310	TRP	2.4
1	C	194	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	80	LEU	2.3
1	A	311	HIS	2.3
1	C	193	LYS	2.3
1	A	269	CYS	2.3
1	C	176	PRO	2.3
1	C	234	LYS	2.3
1	C	164	VAL	2.3
1	B	262	ARG	2.3
1	C	197	ARG	2.3
1	B	267	ASP	2.2
1	C	182	LEU	2.2
1	C	167	ASN	2.2
1	C	168	HIS	2.2
1	C	67	ARG	2.2
1	A	117	HIS	2.1
1	C	290	HIS	2.1
1	C	149	ILE	2.1
1	C	296	PRO	2.1
1	C	196	ASN	2.1
1	C	198	SER	2.1
1	C	309	ASP	2.1
1	C	81	HIS	2.1
1	B	121	VAL	2.1
1	C	240	LYS	2.1
1	C	242	SER	2.1
1	A	277	ALA	2.0
1	C	174	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

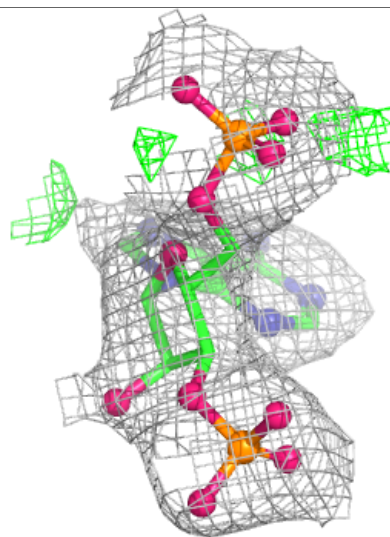
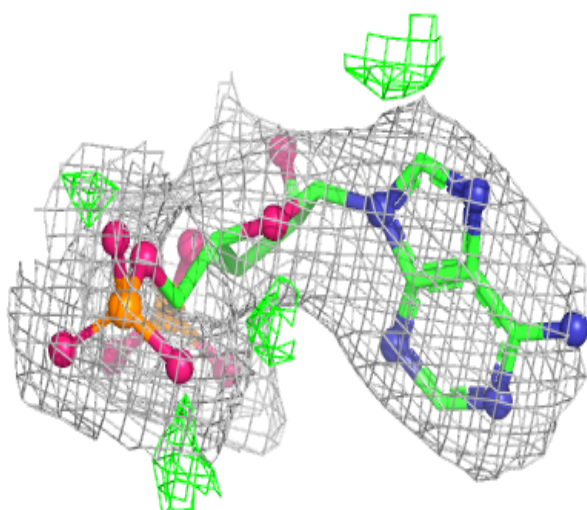
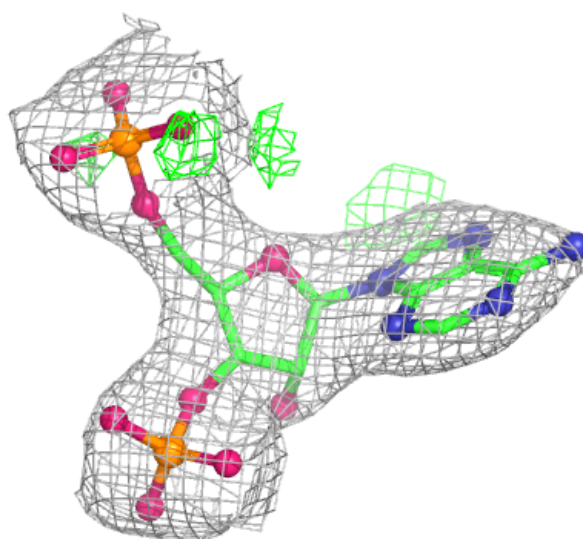
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A3P	A	604	27/27	0.90	0.11	62,70,77,78	0
2	SO4	A	601	5/5	0.93	0.11	86,87,87,87	0
2	SO4	B	602	5/5	0.95	0.08	76,76,76,77	0
3	A3P	A	603	27/27	0.98	0.06	27,33,36,38	0
3	A3P	A	602	27/27	0.98	0.05	27,31,35,38	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.

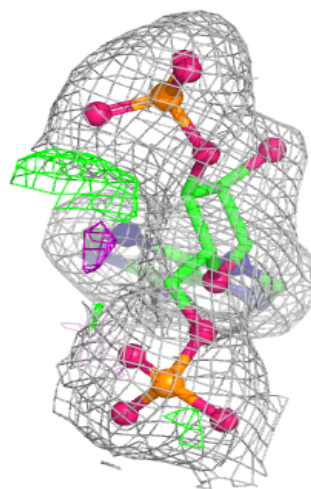
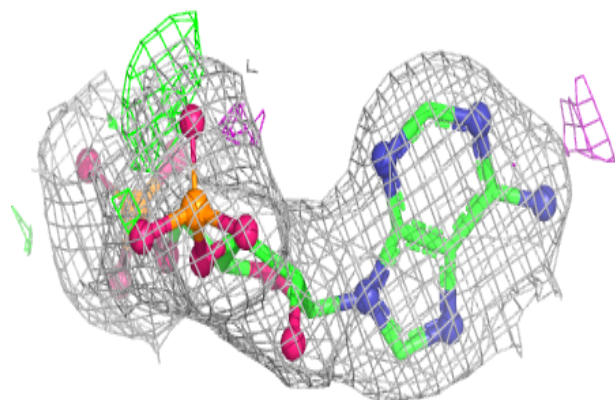
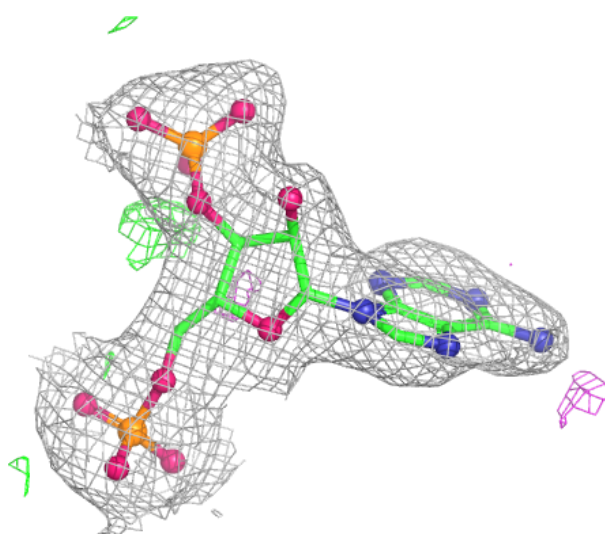
Electron density around A3P A 604:

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



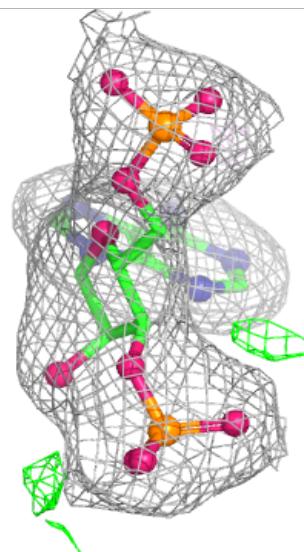
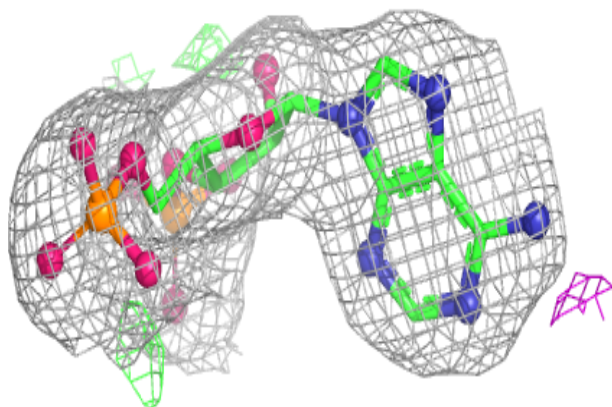
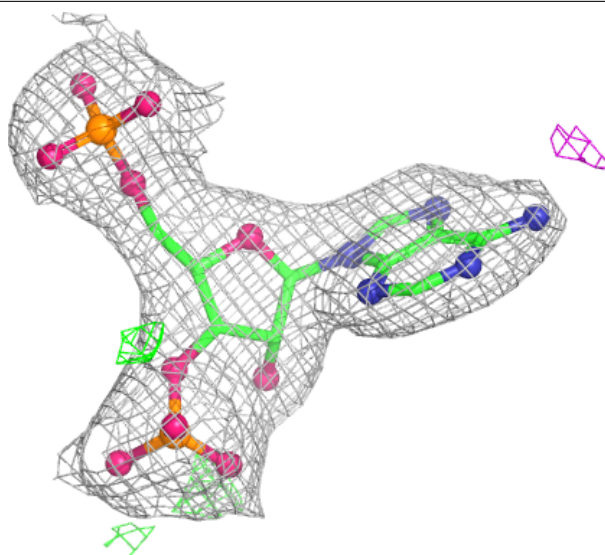
Electron density around A3P A 603:

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



Electron density around A3P A 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.