



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:20 am BST

PDB ID : 3AP3  
Title : Crystal structure of human tyrosylprotein sulfotransferase-2 complexed with PAP  
Authors : Teramoto, T.; Fujikawa, Y.; Kawaguchi, Y.; Kurogi, K.; Soejima, M.; Adachi, R.; Nakanishi, Y.; Mishiro-Sato, E.; Liu, M.-C.; Sakakibara, Y.; Suiko, M.; Kimura, M.; Kakuta, Y.  
Deposited on : 2010-10-09  
Resolution : 3.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

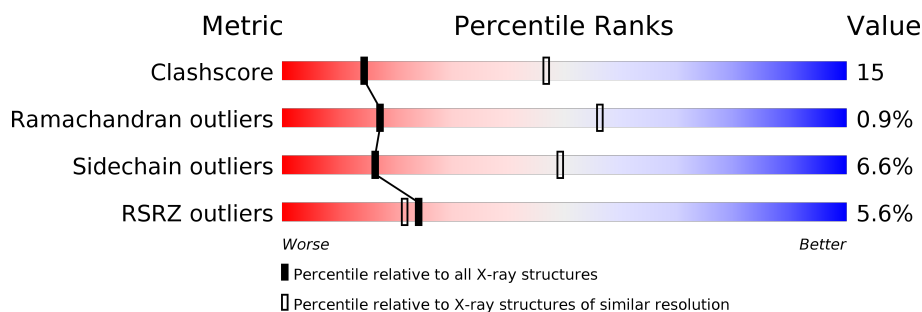
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	355	<div> <div>3%</div> <div>54%</div> <div>23%</div> <div>•</div> <div>21%</div> </div>
1	B	355	<div> <div>11%</div> <div>50%</div> <div>28%</div> <div>•</div> <div>20%</div> </div>
1	C	355	<div> <div>2%</div> <div>56%</div> <div>22%</div> <div>•</div> <div>19%</div> </div>
1	D	355	<div> <div>2%</div> <div>55%</div> <div>23%</div> <div>•</div> <div>18%</div> </div>

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
2	A3P	B	1	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9142 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 Protein-tyrosine sulfotransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2220	1418	390	396	16			
1	B	285	Total	C	N	O	S	0	1	0
			2250	1437	399	398	16			
1	C	286	Total	C	N	O	S	0	1	0
			2261	1441	402	402	16			
1	D	292	Total	C	N	O	S	0	1	0
			2303	1468	408	411	16			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP O60704
A	24	GLY	-	EXPRESSION TAG	UNP O60704
A	25	SER	-	EXPRESSION TAG	UNP O60704
A	26	SER	-	EXPRESSION TAG	UNP O60704
A	27	HIS	-	EXPRESSION TAG	UNP O60704
A	28	HIS	-	EXPRESSION TAG	UNP O60704
A	29	HIS	-	EXPRESSION TAG	UNP O60704
A	30	HIS	-	EXPRESSION TAG	UNP O60704
A	31	HIS	-	EXPRESSION TAG	UNP O60704
A	32	HIS	-	EXPRESSION TAG	UNP O60704
A	33	SER	-	EXPRESSION TAG	UNP O60704
A	34	SER	-	EXPRESSION TAG	UNP O60704
A	35	GLY	-	EXPRESSION TAG	UNP O60704
A	36	VAL	-	EXPRESSION TAG	UNP O60704
A	37	PRO	-	EXPRESSION TAG	UNP O60704
A	38	ARG	-	EXPRESSION TAG	UNP O60704
A	39	GLY	-	EXPRESSION TAG	UNP O60704
A	40	SER	-	EXPRESSION TAG	UNP O60704
A	41	HIS	-	EXPRESSION TAG	UNP O60704
A	42	MET	-	EXPRESSION TAG	UNP O60704
A	61	VAL	GLU	CONFLICT	UNP O60704

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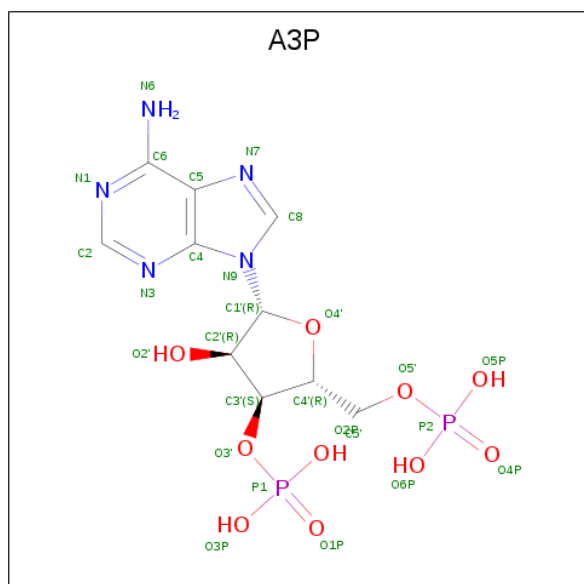
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	MET	-	EXPRESSION TAG	UNP O60704
B	24	GLY	-	EXPRESSION TAG	UNP O60704
B	25	SER	-	EXPRESSION TAG	UNP O60704
B	26	SER	-	EXPRESSION TAG	UNP O60704
B	27	HIS	-	EXPRESSION TAG	UNP O60704
B	28	HIS	-	EXPRESSION TAG	UNP O60704
B	29	HIS	-	EXPRESSION TAG	UNP O60704
B	30	HIS	-	EXPRESSION TAG	UNP O60704
B	31	HIS	-	EXPRESSION TAG	UNP O60704
B	32	HIS	-	EXPRESSION TAG	UNP O60704
B	33	SER	-	EXPRESSION TAG	UNP O60704
B	34	SER	-	EXPRESSION TAG	UNP O60704
B	35	GLY	-	EXPRESSION TAG	UNP O60704
B	36	VAL	-	EXPRESSION TAG	UNP O60704
B	37	PRO	-	EXPRESSION TAG	UNP O60704
B	38	ARG	-	EXPRESSION TAG	UNP O60704
B	39	GLY	-	EXPRESSION TAG	UNP O60704
B	40	SER	-	EXPRESSION TAG	UNP O60704
B	41	HIS	-	EXPRESSION TAG	UNP O60704
B	42	MET	-	EXPRESSION TAG	UNP O60704
B	61	VAL	GLU	CONFLICT	UNP O60704
C	23	MET	-	EXPRESSION TAG	UNP O60704
C	24	GLY	-	EXPRESSION TAG	UNP O60704
C	25	SER	-	EXPRESSION TAG	UNP O60704
C	26	SER	-	EXPRESSION TAG	UNP O60704
C	27	HIS	-	EXPRESSION TAG	UNP O60704
C	28	HIS	-	EXPRESSION TAG	UNP O60704
C	29	HIS	-	EXPRESSION TAG	UNP O60704
C	30	HIS	-	EXPRESSION TAG	UNP O60704
C	31	HIS	-	EXPRESSION TAG	UNP O60704
C	32	HIS	-	EXPRESSION TAG	UNP O60704
C	33	SER	-	EXPRESSION TAG	UNP O60704
C	34	SER	-	EXPRESSION TAG	UNP O60704
C	35	GLY	-	EXPRESSION TAG	UNP O60704
C	36	VAL	-	EXPRESSION TAG	UNP O60704
C	37	PRO	-	EXPRESSION TAG	UNP O60704
C	38	ARG	-	EXPRESSION TAG	UNP O60704
C	39	GLY	-	EXPRESSION TAG	UNP O60704
C	40	SER	-	EXPRESSION TAG	UNP O60704
C	41	HIS	-	EXPRESSION TAG	UNP O60704
C	42	MET	-	EXPRESSION TAG	UNP O60704
C	61	VAL	GLU	CONFLICT	UNP O60704

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Chain	Residue	Modelled	Actual	Comment	Reference
D	23	MET	-	EXPRESSION TAG	UNP O60704
D	24	GLY	-	EXPRESSION TAG	UNP O60704
D	25	SER	-	EXPRESSION TAG	UNP O60704
D	26	SER	-	EXPRESSION TAG	UNP O60704
D	27	HIS	-	EXPRESSION TAG	UNP O60704
D	28	HIS	-	EXPRESSION TAG	UNP O60704
D	29	HIS	-	EXPRESSION TAG	UNP O60704
D	30	HIS	-	EXPRESSION TAG	UNP O60704
D	31	HIS	-	EXPRESSION TAG	UNP O60704
D	32	HIS	-	EXPRESSION TAG	UNP O60704
D	33	SER	-	EXPRESSION TAG	UNP O60704
D	34	SER	-	EXPRESSION TAG	UNP O60704
D	35	GLY	-	EXPRESSION TAG	UNP O60704
D	36	VAL	-	EXPRESSION TAG	UNP O60704
D	37	PRO	-	EXPRESSION TAG	UNP O60704
D	38	ARG	-	EXPRESSION TAG	UNP O60704
D	39	GLY	-	EXPRESSION TAG	UNP O60704
D	40	SER	-	EXPRESSION TAG	UNP O60704
D	41	HIS	-	EXPRESSION TAG	UNP O60704
D	42	MET	-	EXPRESSION TAG	UNP O60704
D	61	VAL	GLU	CONFLICT	UNP O60704

- Molecule 2 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

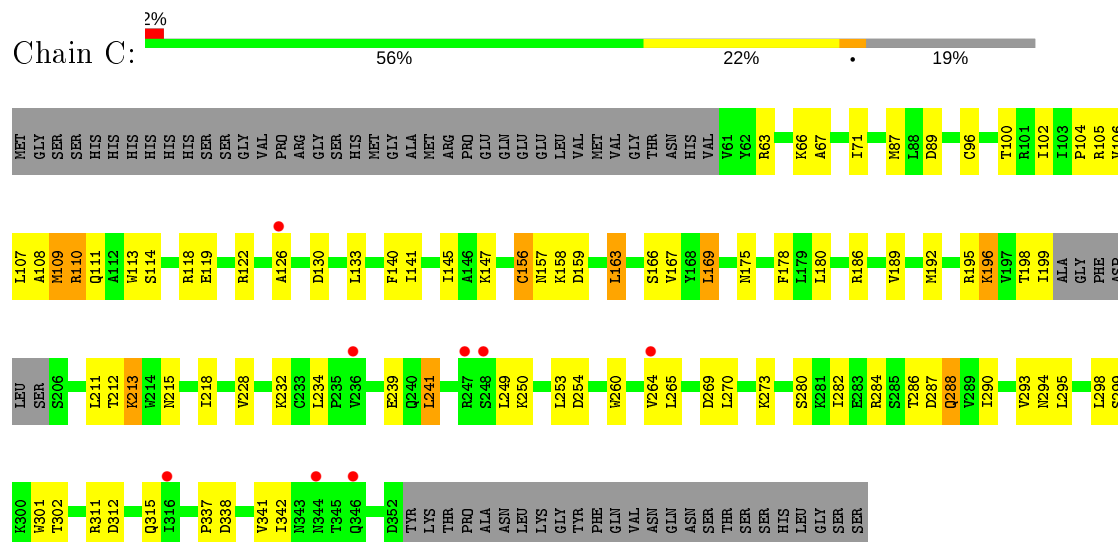


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

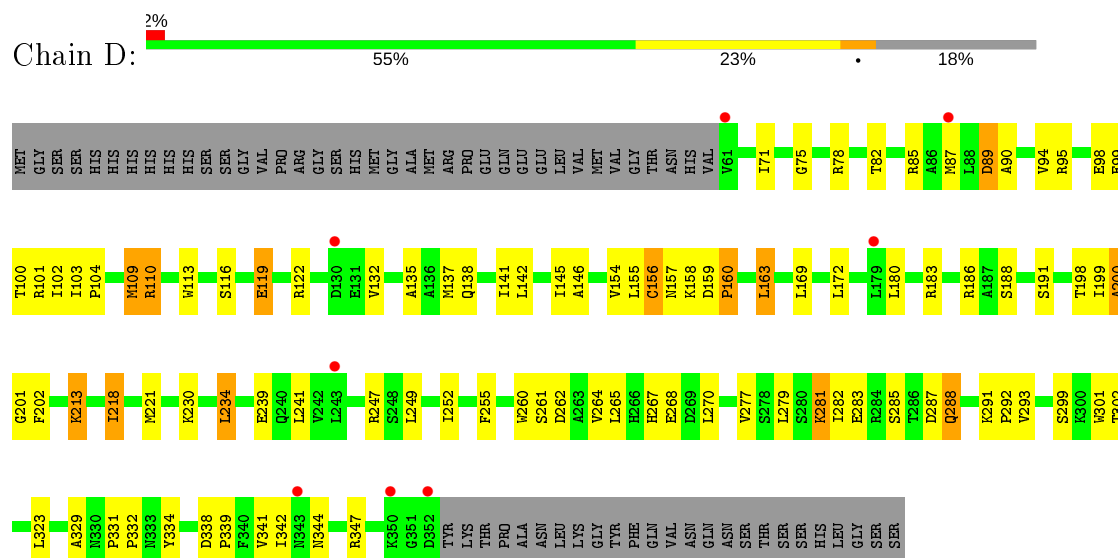




• Molecule 1: Protein-tyrosine sulfotransferase 2



• Molecule 1: Protein-tyrosine sulfotransferase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.43 Å   81.33 Å   226.66 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.50 – 3.50 48.50 – 3.52	Depositor EDS
% Data completeness (in resolution range)	67.1 (48.50-3.50) 64.2 (48.50-3.52)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.22 (at 3.48 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.290   ,   0.371 0.277   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtriage
Anisotropy	1.733	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A3P

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	0.67	3/2272 (0.1%)	0.65	1/3078 (0.0%)
1	B	0.79	4/2301 (0.2%)	0.68	0/3111
1	C	0.63	1/2312 (0.0%)	0.67	2/3128 (0.1%)
1	D	0.58	0/2356	0.69	6/3189 (0.2%)
All	All	0.67	8/9241 (0.1%)	0.67	9/12506 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247[A]	ARG	CZ-NH1	-7.16	1.23	1.33
1	B	247[B]	ARG	CZ-NH1	-7.16	1.23	1.33
1	A	328	TYR	CG-CD2	6.02	1.47	1.39
1	A	328	TYR	CE1-CZ	5.49	1.45	1.38
1	A	328	TYR	CE2-CZ	5.38	1.45	1.38
1	C	63	ARG	CG-CD	-5.26	1.38	1.51
1	B	247[A]	ARG	NE-CZ	-5.19	1.26	1.33
1	B	247[B]	ARG	NE-CZ	-5.19	1.26	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247[A]	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	D	247[B]	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	C	63	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	D	247[A]	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	D	247[B]	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	C	284	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	D	247[A]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	D	247[B]	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	338	ASP	CB-CG-OD1	5.05	122.84	118.30

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	2220	0	2260	75	0
1	B	2250	0	2298	86	0
1	C	2261	0	2315	72	0
1	D	2303	0	2353	77	0
2	A	27	0	11	6	0
2	B	27	0	11	4	0
2	C	27	0	11	3	0
2	D	27	0	11	4	0
All	All	9142	0	9270	284	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 15.

All (284) 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:285:SER:OG	2:A:1:A3P:H5'2	1.66	0.94
1:D:299:SER:O	1:D:302:THR:HG22	1.73	0.88
1:B:104:PRO:HA	1:B:107:LEU:HD12	1.57	0.86
1:B:71:ILE:HB	1:B:156:CYS:HB2	1.58	0.85
1:A:249:LEU:HG	1:A:264:VAL:HG11	1.63	0.81
1:A:199:ILE:HG22	1:A:200:ALA:H	1.46	0.80
1:A:71:ILE:HB	1:A:156:CYS:HB2	1.64	0.77
1:D:71:ILE:HB	1:D:156:CYS:HB2	1.67	0.77
1:C:239:GLU:CD	1:C:239:GLU:H	1.88	0.76
1:C:311:ARG:NH1	1:C:312:ASP:OD2	2.19	0.75
1:C:71:ILE:HB	1:C:156:CYS:HB2	1.69	0.74
1:C:288:GLN:HE21	2:C:1:A3P:H2'	1.52	0.74
1:A:199:ILE:HG22	1:A:200:ALA:N	2.03	0.73
1:B:253:LEU:HD13	1:B:260:TRP:HA	1.68	0.73
1:C:282:ILE:HD11	1:D:122:ARG:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ASP:O	1:D:291:LYS:HE2	1.90	0.72
1:A:242:VAL:HG12	1:A:295:LEU:HD23	1.72	0.71
1:A:249:LEU:HG	1:A:264:VAL:CG1	2.19	0.71
1:A:147:LYS:HB2	1:B:132:VAL:HG13	1.71	0.71
1:D:135:ALA:HA	1:D:138:GLN:OE1	1.91	0.70
1:A:102:ILE:HD11	1:B:113:TRP:CH2	2.27	0.70
1:B:106:VAL:HA	1:B:109:MET:SD	2.32	0.70
1:A:78:ARG:HA	2:A:1:A3P:H5'1	1.74	0.68
1:B:299:SER:O	1:B:302:THR:HG22	1.93	0.68
1:A:139:ALA:HB1	1:B:139:ALA:HB1	1.76	0.67
1:A:163:LEU:HD12	1:A:180:LEU:HD13	1.75	0.67
1:C:249:LEU:HG	1:C:264:VAL:CG1	2.24	0.66
1:D:202:PHE:CE2	1:D:213:LYS:HB3	2.31	0.66
1:C:105:ARG:HD3	1:D:113:TRP:HE1	1.61	0.66
1:C:270:LEU:HA	1:C:273:LYS:HD2	1.76	0.66
1:C:113:TRP:CZ3	1:D:102:ILE:HD11	2.30	0.65
1:D:239:GLU:H	1:D:239:GLU:CD	2.00	0.65
1:C:106:VAL:HA	1:C:109:MET:SD	2.36	0.64
1:B:78:ARG:O	1:B:183:ARG:NH1	2.29	0.64
1:B:82:THR:CG2	1:B:289:VAL:HG21	2.27	0.64
1:D:138:GLN:HG3	1:D:172:LEU:HD22	1.79	0.64
1:A:199:ILE:CG2	1:A:200:ALA:H	2.11	0.64
1:C:156:CYS:SG	1:C:157:ASN:N	2.70	0.64
1:A:100:THR:HG23	1:A:157:ASN:HD21	1.63	0.64
1:A:208:ARG:NH2	1:A:312:ASP:OD2	2.30	0.64
1:D:90:ALA:HB1	1:D:270:LEU:HD12	1.80	0.64
1:A:247[A]:ARG:HE	1:A:251:LEU:HD11	1.63	0.63
1:B:152:ALA:HB3	1:B:155:LEU:HD23	1.80	0.63
1:C:169:LEU:HB3	1:C:178:PHE:HZ	1.64	0.63
2:A:1:A3P:O2'	2:A:1:A3P:O2P	2.15	0.63
1:B:101:ARG:HD3	1:C:196:LYS:HG2	1.81	0.63
1:D:103:ILE:N	1:D:104:PRO:HD2	2.14	0.62
1:D:78:ARG:NH1	1:D:285:SER:OG	2.32	0.62
1:A:102:ILE:HD11	1:B:113:TRP:CZ3	2.34	0.62
1:B:239:GLU:H	1:B:239:GLU:CD	2.01	0.62
1:B:156:CYS:SG	1:B:157:ASN:N	2.72	0.61
1:D:78:ARG:O	1:D:183:ARG:NH1	2.31	0.61
1:A:299:SER:O	1:A:302:THR:HG22	2.00	0.61
1:A:101:ARG:NE	1:B:122:ARG:HD3	2.16	0.60
1:C:294:ASN:O	2:C:1:A3P:H2	2.02	0.60
1:B:338:ASP:HB2	1:B:341:VAL:HG23	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LEU:HD12	1:D:180:LEU:HD13	1.84	0.59
1:D:78:ARG:HA	2:D:1:A3P:H5'1	1.84	0.59
1:B:96:CYS:HA	1:B:156:CYS:O	2.01	0.59
2:D:1:A3P:O2'	2:D:1:A3P:O2P	2.18	0.59
1:D:267:HIS:NE2	1:D:292:PRO:HA	2.18	0.59
1:C:299:SER:O	1:C:302:THR:HG22	2.02	0.59
1:B:195:ARG:O	1:B:284:ARG:NH2	2.36	0.58
1:D:338:ASP:HB2	1:D:341:VAL:HG23	1.85	0.58
1:B:102:ILE:O	1:B:105:ARG:HB3	2.03	0.58
1:A:102:ILE:HD11	1:B:113:TRP:CZ2	2.38	0.58
1:D:344:ASN:OD1	1:D:347:ARG:NH1	2.33	0.58
1:C:315:GLN:N	1:C:315:GLN:CD	2.56	0.58
1:A:281:LYS:O	1:A:281:LYS:HG3	2.03	0.58
1:C:186:ARG:HD2	1:C:301:TRP:CZ3	2.39	0.57
1:B:295:LEU:HD21	1:B:337:PRO:HB3	1.86	0.57
1:A:94:VAL:HG22	1:A:154:VAL:HB	1.85	0.57
1:D:218:ILE:HD12	1:D:323:LEU:HD11	1.87	0.57
1:C:249:LEU:HG	1:C:264:VAL:HG11	1.86	0.56
1:B:245:PRO:HD2	1:B:338:ASP:OD2	2.04	0.56
1:C:228:VAL:CG1	1:C:232:LYS:HB2	2.36	0.56
1:B:110:ARG:HA	1:B:113:TRP:CE3	2.41	0.55
1:C:249:LEU:HG	1:C:264:VAL:HG13	1.87	0.55
1:D:186:ARG:HD2	1:D:301:TRP:CZ3	2.42	0.55
1:A:302:THR:HG21	1:A:331:PRO:HD3	1.89	0.55
1:B:204:LEU:HD11	1:C:199:ILE:HG22	1.88	0.54
1:B:182:VAL:HG11	1:B:323:LEU:HD22	1.90	0.54
1:B:190:HIS:CE1	1:B:194:THR:HG21	2.42	0.54
1:C:106:VAL:HA	1:C:109:MET:CE	2.38	0.54
1:C:113:TRP:CH2	1:D:102:ILE:HD11	2.41	0.54
1:D:95:ARG:NH1	1:D:146:ALA:O	2.41	0.54
1:D:249:LEU:HG	1:D:264:VAL:CG1	2.38	0.54
1:A:89:ASP:OD1	1:A:95:ARG:HG2	2.08	0.54
1:C:253:LEU:HD12	1:C:260:TRP:CE3	2.43	0.54
1:C:264:VAL:HG12	1:C:265:LEU:HG	1.90	0.54
1:B:269:ASP:O	1:B:273:LYS:HD2	2.08	0.54
1:C:67:ALA:O	1:C:175:ASN:HB2	2.08	0.54
1:D:110:ARG:HD3	1:D:110:ARG:C	2.28	0.54
1:B:212:THR:O	1:B:215:ASN:HB3	2.08	0.54
1:A:110:ARG:C	1:A:110:ARG:HD3	2.29	0.53
1:D:90:ALA:HB1	1:D:270:LEU:CD1	2.38	0.53
1:B:189:VAL:HA	1:B:192:MET:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HG	1:B:264:VAL:HG13	1.90	0.53
1:D:249:LEU:O	1:D:252:ILE:HB	2.08	0.53
1:A:249:LEU:HA	1:A:252:ILE:HD12	1.90	0.53
1:D:156:CYS:SG	1:D:157:ASN:N	2.82	0.53
1:A:186:ARG:HD2	1:A:301:TRP:CH2	2.44	0.53
1:A:329:ALA:HB1	1:A:332:PRO:HA	1.91	0.52
1:C:195:ARG:NE	2:C:1:A3P:O1P	2.42	0.52
1:D:302:THR:HG21	1:D:331:PRO:HD3	1.91	0.52
1:B:179:LEU:HD22	1:B:236:VAL:HG21	1.92	0.52
1:A:103:ILE:N	1:A:104:PRO:HD2	2.25	0.52
1:A:96:CYS:HA	1:A:156:CYS:O	2.09	0.52
1:B:249:LEU:HG	1:B:264:VAL:CG1	2.40	0.52
1:C:169:LEU:HB3	1:C:178:PHE:CZ	2.45	0.51
1:D:100:THR:C	1:D:102:ILE:H	2.12	0.51
1:A:148:HIS:O	1:B:127:GLY:HA3	2.11	0.51
1:A:156:CYS:SG	1:A:157:ASN:N	2.83	0.51
1:B:169:LEU:HB3	1:B:178:PHE:HZ	1.76	0.51
1:B:228:VAL:HG11	1:B:233:CYS:HB2	1.91	0.51
1:A:78:ARG:HA	2:A:1:A3P:C5'	2.40	0.51
1:D:78:ARG:NH2	1:D:288:GLN:HE22	2.09	0.50
1:C:147:LYS:HB2	1:D:132:VAL:HG13	1.93	0.50
1:D:288:GLN:HE21	2:D:1:A3P:H2'	1.76	0.50
1:D:186:ARG:HD2	1:D:301:TRP:CH2	2.46	0.50
1:A:185:GLY:HA3	1:A:214:TRP:CE2	2.46	0.50
1:D:339:PRO:HA	1:D:342:ILE:HD12	1.92	0.50
1:A:288:GLN:HE21	2:A:1:A3P:H2'	1.77	0.50
1:C:110:ARG:HA	1:C:113:TRP:CE3	2.47	0.50
1:A:199:ILE:CG2	1:A:200:ALA:N	2.70	0.49
1:B:253:LEU:HD12	1:B:260:TRP:CE3	2.47	0.49
1:A:253:LEU:O	1:A:257:GLY:N	2.45	0.49
1:A:312:ASP:HB2	1:A:316:ILE:HD11	1.94	0.49
1:B:166:SER:HA	1:B:169:LEU:HB2	1.94	0.49
1:B:250:LYS:N	1:B:260:TRP:HZ3	2.10	0.49
1:C:102:ILE:HD11	1:D:113:TRP:CH2	2.47	0.49
1:D:94:VAL:HG22	1:D:154:VAL:HB	1.93	0.49
1:C:337:PRO:HG2	1:C:342:ILE:HD11	1.95	0.49
1:D:116:SER:OG	1:D:119:GLU:HB3	2.13	0.48
1:D:85:ARG:NH2	1:D:279:LEU:HD23	2.27	0.48
1:A:100:THR:CG2	1:A:157:ASN:HD21	2.27	0.48
1:B:203:ASP:HB3	1:B:209:ASP:OD2	2.14	0.48
1:D:78:ARG:HA	2:D:1:A3P:C5'	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:CD1	1:B:258:ILE:HD12	2.44	0.48
1:B:82:THR:HB	1:B:289:VAL:HG21	1.94	0.48
1:C:228:VAL:HG12	1:C:232:LYS:HB2	1.96	0.48
1:C:250:LYS:O	1:C:254:ASP:HB2	2.13	0.48
1:B:277:VAL:HG12	1:B:279:LEU:HD21	1.95	0.48
1:B:239:GLU:OE1	1:B:325:TYR:OH	2.32	0.48
1:A:212:THR:O	1:A:215:ASN:HB3	2.14	0.47
1:B:108:ALA:O	1:B:111:GLN:HB3	2.13	0.47
1:C:119:GLU:HA	1:C:122:ARG:HD3	1.96	0.47
1:D:249:LEU:HG	1:D:264:VAL:HG13	1.95	0.47
1:C:102:ILE:HD11	1:D:113:TRP:CZ3	2.50	0.47
1:B:204:LEU:HD11	1:C:199:ILE:C	2.34	0.47
1:B:264:VAL:HG12	1:B:265:LEU:HG	1.95	0.47
1:D:75:GLY:HA2	1:D:221:MET:SD	2.54	0.47
1:B:109:MET:HB2	1:B:109:MET:HE2	1.65	0.47
1:C:126:ALA:HB1	1:D:99:GLU:O	2.14	0.47
1:D:299:SER:HG	1:D:334:TYR:HE2	1.62	0.47
1:A:109:MET:HB2	1:A:109:MET:HE2	1.56	0.47
1:A:109:MET:HB3	1:A:113:TRP:CZ2	2.50	0.47
1:A:90:ALA:HB1	1:A:270:LEU:HD12	1.95	0.47
1:D:159:ASP:O	1:D:160:PRO:C	2.53	0.47
1:B:106:VAL:HA	1:B:109:MET:CE	2.45	0.47
1:B:138:GLN:HG3	1:B:172:LEU:HD22	1.96	0.47
1:B:87:MET:CE	1:B:241:LEU:HD21	2.45	0.46
1:D:249:LEU:HA	1:D:252:ILE:HD12	1.97	0.46
1:C:311:ARG:HH11	1:C:312:ASP:CG	2.17	0.46
1:A:102:ILE:HD11	1:B:113:TRP:CE2	2.50	0.46
1:B:277:VAL:HG12	1:B:279:LEU:CD2	2.44	0.46
1:D:89:ASP:HB3	1:D:277:VAL:HA	1.96	0.46
1:D:145:ILE:HG22	1:D:155:LEU:HD13	1.98	0.46
1:A:319:MET:O	1:A:320:LEU:C	2.54	0.46
1:B:289:VAL:HG23	2:B:1:A3P:H8	1.98	0.46
1:B:71:ILE:HD12	1:B:156:CYS:HB2	1.98	0.46
1:A:109:MET:HE3	1:A:113:TRP:CH2	2.51	0.46
1:C:212:THR:O	1:C:215:ASN:HB3	2.16	0.46
1:A:109:MET:CE	1:A:113:TRP:CH2	2.99	0.46
1:B:102:ILE:HD12	1:B:105:ARG:HD2	1.98	0.46
1:C:100:THR:C	1:C:102:ILE:H	2.19	0.46
1:D:100:THR:HB	1:D:102:ILE:HG22	1.97	0.46
1:D:262:ASP:C	1:D:264:VAL:N	2.69	0.46
1:B:339:PRO:HA	1:B:342:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:HA	1:C:122:ARG:HB2	1.97	0.45
1:C:163:LEU:HD12	1:C:180:LEU:HB2	1.98	0.45
1:D:78:ARG:HH22	1:D:288:GLN:HE22	1.63	0.45
1:B:68:MET:HB2	1:B:69:PRO:CD	2.47	0.45
1:D:110:ARG:HA	1:D:113:TRP:CE3	2.52	0.45
1:D:329:ALA:HB1	1:D:332:PRO:HA	1.99	0.45
1:B:256:LEU:HD13	1:B:258:ILE:CD1	2.47	0.45
1:D:98:GLU:HB3	1:D:283:GLU:OE2	2.15	0.45
1:D:249:LEU:HD13	1:D:252:ILE:HD12	1.99	0.45
1:A:102:ILE:HD11	1:B:113:TRP:CE3	2.51	0.45
1:C:118:ARG:HG2	1:C:122:ARG:HD2	1.98	0.45
1:C:108:ALA:O	1:C:111:GLN:HB3	2.17	0.45
1:A:186:ARG:HD2	1:A:301:TRP:CZ3	2.51	0.45
1:D:100:THR:O	1:D:101:ARG:HB2	2.17	0.45
1:A:306:PRO:O	1:A:310:VAL:HG23	2.17	0.44
1:D:199:ILE:HG22	1:D:200:ALA:N	2.31	0.44
1:A:109:MET:CE	1:A:113:TRP:HH2	2.30	0.44
1:A:264:VAL:HG12	1:A:265:LEU:HG	1.99	0.44
1:B:177:LYS:HE2	1:B:255:PHE:O	2.17	0.44
1:C:338:ASP:HB2	1:C:341:VAL:HG23	1.98	0.44
1:B:169:LEU:HD23	1:B:178:PHE:HE1	1.83	0.44
1:D:188:SER:O	1:D:191:SER:HB3	2.18	0.44
1:D:141:ILE:O	1:D:142:LEU:C	2.54	0.44
1:A:285:SER:HG	2:A:1:A3P:H5'2	1.78	0.44
1:A:282:ILE:HD11	1:B:122:ARG:HA	2.00	0.44
1:C:228:VAL:CG1	1:C:232:LYS:CB	2.95	0.44
1:C:282:ILE:HD12	1:D:122:ARG:HG3	2.00	0.44
1:A:148:HIS:HA	1:B:127:GLY:O	2.18	0.44
1:B:193:ILE:HG21	1:B:207:TYR:CE2	2.53	0.44
1:B:203:ASP:HB2	1:C:213:LYS:NZ	2.33	0.44
1:A:159:ASP:O	1:A:160:PRO:C	2.55	0.44
1:A:253:LEU:HA	1:A:256:LEU:HB2	1.99	0.44
1:A:325:TYR:O	1:A:327:PRO:HD3	2.18	0.43
1:B:113:TRP:O	1:B:116:SER:HB3	2.19	0.43
1:A:274:PRO:C	1:A:276:GLY:H	2.21	0.43
1:B:82:THR:CB	1:B:289:VAL:HG21	2.48	0.43
1:C:105:ARG:HD3	1:D:113:TRP:NE1	2.31	0.43
1:D:292:PRO:HG3	1:D:347:ARG:HH21	1.83	0.43
1:B:169:LEU:HB3	1:B:178:PHE:CZ	2.54	0.43
1:D:264:VAL:HG12	1:D:265:LEU:HG	1.99	0.43
1:B:161:PHE:CD1	1:B:164:LYS:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:O	1:C:298:LEU:HG	2.19	0.43
1:D:137:MET:O	1:D:138:GLN:C	2.56	0.43
1:D:109:MET:HE2	1:D:109:MET:HB2	1.54	0.43
1:B:135:ALA:HA	1:B:138:GLN:OE1	2.19	0.43
1:B:204:LEU:CD1	1:C:199:ILE:HG22	2.48	0.43
1:B:203:ASP:HB3	1:B:209:ASP:CG	2.38	0.43
1:A:242:VAL:O	1:A:341:VAL:HG11	2.19	0.43
1:C:109:MET:HE2	1:C:109:MET:HB2	1.70	0.42
1:D:234:LEU:HB2	1:D:255:PHE:CE1	2.54	0.42
1:D:87:MET:HE3	1:D:249:LEU:HD21	2.00	0.42
1:B:289:VAL:HA	2:B:1:A3P:N7	2.34	0.42
1:B:80:GLY:N	2:B:1:A3P:O5P	2.52	0.42
1:C:104:PRO:HA	1:C:107:LEU:HD12	2.02	0.42
1:C:189:VAL:HG21	1:C:211:LEU:HG	2.02	0.42
1:A:133:LEU:O	1:A:137:MET:HG2	2.19	0.42
1:A:190:HIS:CE1	1:A:194:THR:HG21	2.54	0.42
1:A:100:THR:O	1:A:101:ARG:HB2	2.19	0.42
1:A:328:TYR:O	1:A:330:ASN:ND2	2.49	0.42
1:B:103:ILE:N	1:B:104:PRO:HD2	2.34	0.42
1:B:329:ALA:HB1	1:B:332:PRO:HA	2.02	0.42
1:B:87:MET:HE1	1:B:241:LEU:HD21	2.02	0.42
1:C:166:SER:O	1:C:167:VAL:C	2.58	0.42
1:C:287:ASP:HA	1:C:290:ILE:HG12	2.02	0.42
1:A:100:THR:C	1:A:102:ILE:H	2.23	0.42
1:D:281:LYS:HG3	1:D:282:ILE:HG23	2.01	0.42
1:C:130:ASP:O	1:C:133:LEU:HB2	2.20	0.42
1:C:280:SER:O	1:C:286:THR:OG1	2.26	0.42
1:D:199:ILE:O	1:D:201:GLY:N	2.53	0.42
1:D:82:THR:O	1:D:85:ARG:HG3	2.20	0.42
1:A:249:LEU:HA	1:A:249:LEU:HD13	1.90	0.42
1:C:141:ILE:O	1:C:145:ILE:HG13	2.20	0.42
1:D:260:TRP:CG	1:D:261:SER:N	2.88	0.42
1:A:195:ARG:O	1:A:284:ARG:NH2	2.54	0.41
1:A:82:THR:HG21	1:A:285:SER:O	2.21	0.41
1:A:102:ILE:HA	1:A:102:ILE:HD12	1.78	0.41
1:B:103:ILE:O	1:B:106:VAL:HG22	2.19	0.41
1:B:189:VAL:HG21	1:B:211:LEU:HG	2.02	0.41
1:C:102:ILE:HD12	1:C:102:ILE:HA	1.89	0.41
1:C:299:SER:HA	1:C:301:TRP:CD1	2.55	0.41
1:C:122:ARG:HA	1:D:282:ILE:HD11	2.02	0.41
1:A:135:ALA:HA	1:A:138:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LEU:HG	1:D:264:VAL:HG11	2.01	0.41
1:B:184:ASP:OD1	1:B:320:LEU:HD22	2.20	0.41
1:C:106:VAL:HG11	1:C:140:PHE:CE2	2.56	0.41
1:B:78:ARG:HA	2:B:1:A3P:H5'1	2.03	0.41
1:C:189:VAL:HA	1:C:192:MET:HG2	2.02	0.41
1:C:269:ASP:O	1:C:273:LYS:HD2	2.21	0.41
1:C:87:MET:CE	1:C:241:LEU:HD21	2.51	0.41
1:D:102:ILE:HA	1:D:102:ILE:HD12	1.89	0.41
1:D:268:GLU:CD	1:D:292:PRO:HB3	2.41	0.41
1:A:242:VAL:CG1	1:A:295:LEU:HD23	2.48	0.41
1:C:239:GLU:CD	1:C:239:GLU:N	2.67	0.41
1:A:145:ILE:HA	1:A:148:HIS:HD2	1.86	0.41
1:A:306:PRO:HB2	1:A:309:VAL:HG23	2.03	0.41
1:B:186:ARG:HD2	1:B:301:TRP:CZ3	2.56	0.41
1:B:305:ILE:HB	1:B:310:VAL:HG22	2.01	0.41
1:A:131:GLU:CD	1:A:131:GLU:H	2.25	0.41
1:B:253:LEU:HB3	1:B:258:ILE:O	2.20	0.41
1:A:249:LEU:HG	1:A:264:VAL:HG13	2.01	0.40
1:B:89:ASP:O	1:B:276:GLY:HA2	2.20	0.40
1:C:109:MET:HB3	1:C:113:TRP:CZ2	2.56	0.40
1:C:166:SER:HA	1:C:169:LEU:HB2	2.02	0.40
1:C:96:CYS:HA	1:C:156:CYS:O	2.20	0.40
1:C:109:MET:SD	1:D:109:MET:SD	3.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	279/355 (79%)	250 (90%)	27 (10%)	2 (1%)	22 61
1	B	280/355 (79%)	259 (92%)	19 (7%)	2 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	283/355 (80%)	260 (92%)	20 (7%)	3 (1%)	14	52
1	D	291/355 (82%)	263 (90%)	25 (9%)	3 (1%)	15	54
All	All	1133/1420 (80%)	1032 (91%)	91 (8%)	10 (1%)	17	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	LYS
1	C	66	LYS
1	D	200	ALA
1	A	293	VAL
1	B	293	VAL
1	A	200	ALA
1	C	293	VAL
1	C	163	LEU
1	D	293	VAL
1	D	160	PRO

### 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	242/304 (80%)	225 (93%)	17 (7%)	15	46
1	B	244/304 (80%)	227 (93%)	17 (7%)	15	46
1	C	247/304 (81%)	232 (94%)	15 (6%)	18	51
1	D	251/304 (83%)	235 (94%)	16 (6%)	17	50
All	All	984/1216 (81%)	919 (93%)	65 (7%)	16	49

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	114	SER
1	A	156	CYS
1	A	158	LYS
1	A	163	LEU
1	A	169	LEU
1	A	196	LYS
1	A	198	THR
1	A	205	SER
1	A	213	LYS
1	A	218	ILE
1	A	234	LEU
1	A	241	LEU
1	A	281	LYS
1	A	285	SER
1	A	288	GLN
1	B	64	TYR
1	B	89	ASP
1	B	109	MET
1	B	110	ARG
1	B	114	SER
1	B	118	ARG
1	B	148	HIS
1	B	156	CYS
1	B	158	LYS
1	B	163	LEU
1	B	169	LEU
1	B	203	ASP
1	B	213	LYS
1	B	218	ILE
1	B	230	LYS
1	B	234	LEU
1	B	241	LEU
1	C	89	ASP
1	C	109	MET
1	C	110	ARG
1	C	114	SER
1	C	156	CYS
1	C	158	LYS
1	C	159	ASP
1	C	169	LEU
1	C	196	LYS
1	C	198	THR

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Mol	Chain	Res	Type
1	C	213	LYS
1	C	218	ILE
1	C	234	LEU
1	C	241	LEU
1	C	288	GLN
1	D	89	ASP
1	D	109	MET
1	D	110	ARG
1	D	119	GLU
1	D	156	CYS
1	D	158	LYS
1	D	163	LEU
1	D	169	LEU
1	D	198	THR
1	D	213	LYS
1	D	218	ILE
1	D	230	LYS
1	D	234	LEU
1	D	241	LEU
1	D	281	LYS
1	D	288	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	157	ASN
1	A	175	ASN
1	A	190	HIS
1	A	215	ASN
1	A	288	GLN
1	A	294	ASN
1	A	333	ASN
1	B	175	ASN
1	B	190	HIS
1	B	215	ASN
1	B	294	ASN
1	B	304	HIS
1	B	333	ASN
1	C	111	GLN
1	C	157	ASN
1	C	175	ASN

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Mol	Chain	Res	Type
1	C	215	ASN
1	C	288	GLN
1	C	294	ASN
1	C	304	HIS
1	C	333	ASN
1	D	111	GLN
1	D	148	HIS
1	D	157	ASN
1	D	175	ASN
1	D	190	HIS
1	D	215	ASN
1	D	288	GLN
1	D	294	ASN
1	D	333	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	A3P	C	1	-	26,29,29	1.18	3 (11%)	31,45,45	1.42	5 (16%)
2	A3P	D	1	-	26,29,29	1.05	1 (3%)	31,45,45	1.57	6 (19%)
2	A3P	A	1	-	26,29,29	1.08	2 (7%)	31,45,45	1.75	8 (25%)
2	A3P	B	1	-	26,29,29	1.39	5 (19%)	31,45,45	1.43	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A3P	C	1	-	-	2/11/31/31	0/3/3/3
2	A3P	D	1	-	-	3/11/31/31	0/3/3/3
2	A3P	A	1	-	-	5/11/31/31	0/3/3/3
2	A3P	B	1	-	-	4/11/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	A3P	P1-O3'	3.42	1.65	1.59
2	B	1	A3P	C5-C4	3.11	1.49	1.40
2	B	1	A3P	O4'-C1'	2.71	1.44	1.41
2	C	1	A3P	C5-C4	2.71	1.48	1.40
2	C	1	A3P	P1-O3'	2.59	1.64	1.59
2	A	1	A3P	C5-C4	2.57	1.47	1.40
2	D	1	A3P	C5-C4	2.51	1.47	1.40
2	C	1	A3P	O4'-C1'	2.45	1.44	1.41
2	A	1	A3P	C2'-C1'	-2.23	1.50	1.53
2	B	1	A3P	C2-N3	2.22	1.35	1.32
2	B	1	A3P	C4-N3	2.16	1.38	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	A3P	O6P-P2-O5'	-4.83	93.88	106.73
2	A	1	A3P	N3-C2-N1	-4.53	121.61	128.68
2	D	1	A3P	O6P-P2-O5'	-3.60	97.16	106.73
2	D	1	A3P	N3-C2-N1	-3.58	123.08	128.68
2	B	1	A3P	N3-C2-N1	-3.48	123.24	128.68
2	C	1	A3P	C3'-C2'-C1'	3.08	106.70	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	A3P	N3-C2-N1	-2.95	124.06	128.68
2	C	1	A3P	O6P-P2-O5'	-2.95	98.89	106.73
2	B	1	A3P	C3'-C2'-C1'	2.93	106.38	99.89
2	D	1	A3P	O3'-P1-O1P	-2.90	98.20	109.39
2	A	1	A3P	N6-C6-N1	2.85	124.49	118.57
2	A	1	A3P	C2-N1-C6	2.85	123.62	118.75
2	B	1	A3P	C4-C5-N7	-2.52	106.78	109.40
2	A	1	A3P	O6P-P2-O4P	2.51	120.52	110.68
2	D	1	A3P	O6P-P2-O5P	2.41	116.84	107.64
2	C	1	A3P	C4-C5-N7	-2.38	106.92	109.40
2	B	1	A3P	O4'-C4'-C3'	2.37	109.94	104.87
2	A	1	A3P	O3'-P1-O1P	-2.28	100.60	109.39
2	A	1	A3P	O6P-P2-O5P	2.24	116.19	107.64
2	C	1	A3P	O3'-P1-O1P	-2.20	100.92	109.39
2	A	1	A3P	O4'-C1'-C2'	-2.14	103.80	106.93
2	D	1	A3P	C2-N1-C6	2.11	122.37	118.75
2	D	1	A3P	C3'-C2'-C1'	2.06	104.46	99.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

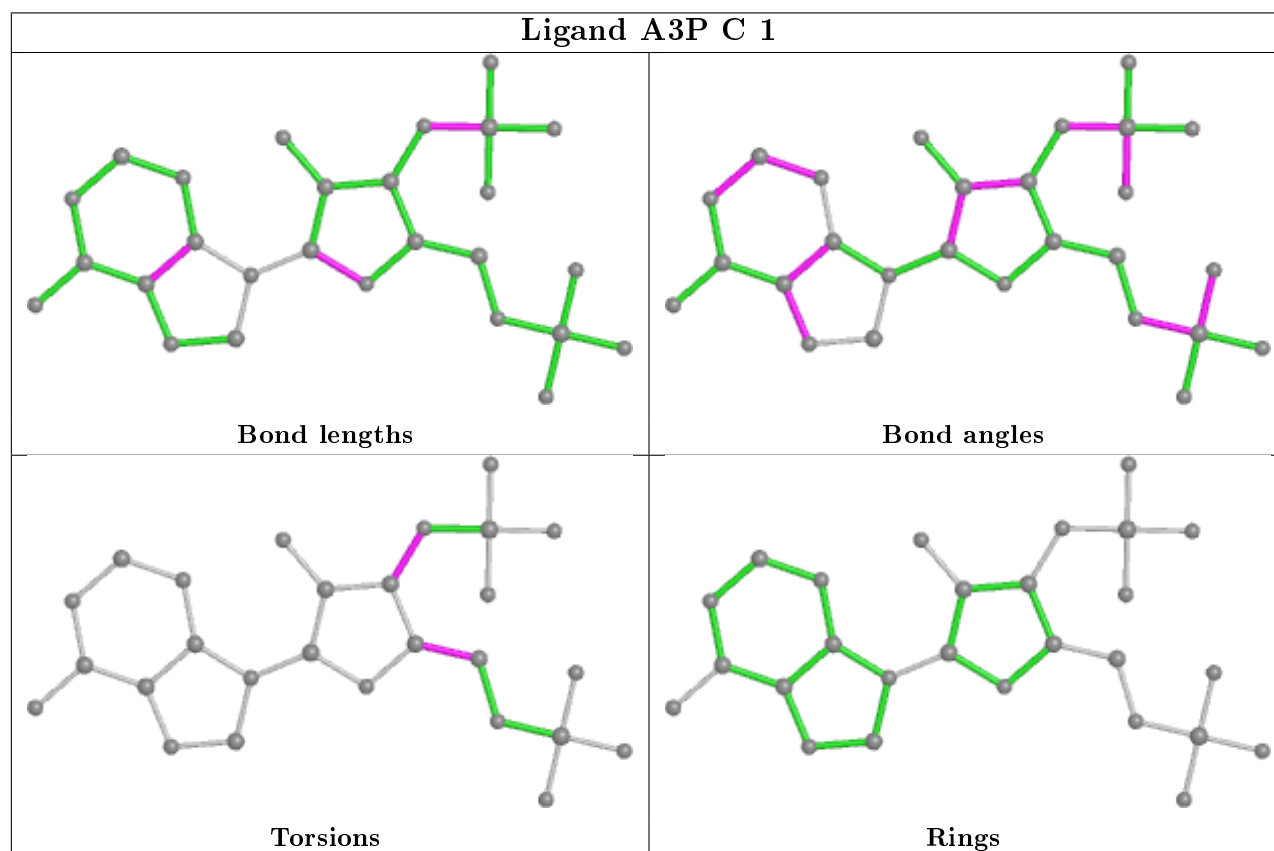
Mol	Chain	Res	Type	Atoms
2	A	1	A3P	C5'-O5'-P2-O5P
2	A	1	A3P	C5'-O5'-P2-O6P
2	B	1	A3P	C5'-O5'-P2-O4P
2	B	1	A3P	C5'-O5'-P2-O5P
2	B	1	A3P	C5'-O5'-P2-O6P
2	C	1	A3P	C3'-C4'-C5'-O5'
2	A	1	A3P	C2'-C3'-O3'-P1
2	D	1	A3P	C2'-C3'-O3'-P1
2	A	1	A3P	C4'-C3'-O3'-P1
2	D	1	A3P	C5'-O5'-P2-O5P
2	D	1	A3P	C4'-C3'-O3'-P1
2	A	1	A3P	C5'-O5'-P2-O4P
2	C	1	A3P	C2'-C3'-O3'-P1
2	B	1	A3P	C2'-C3'-O3'-P1

There are no ring outliers.

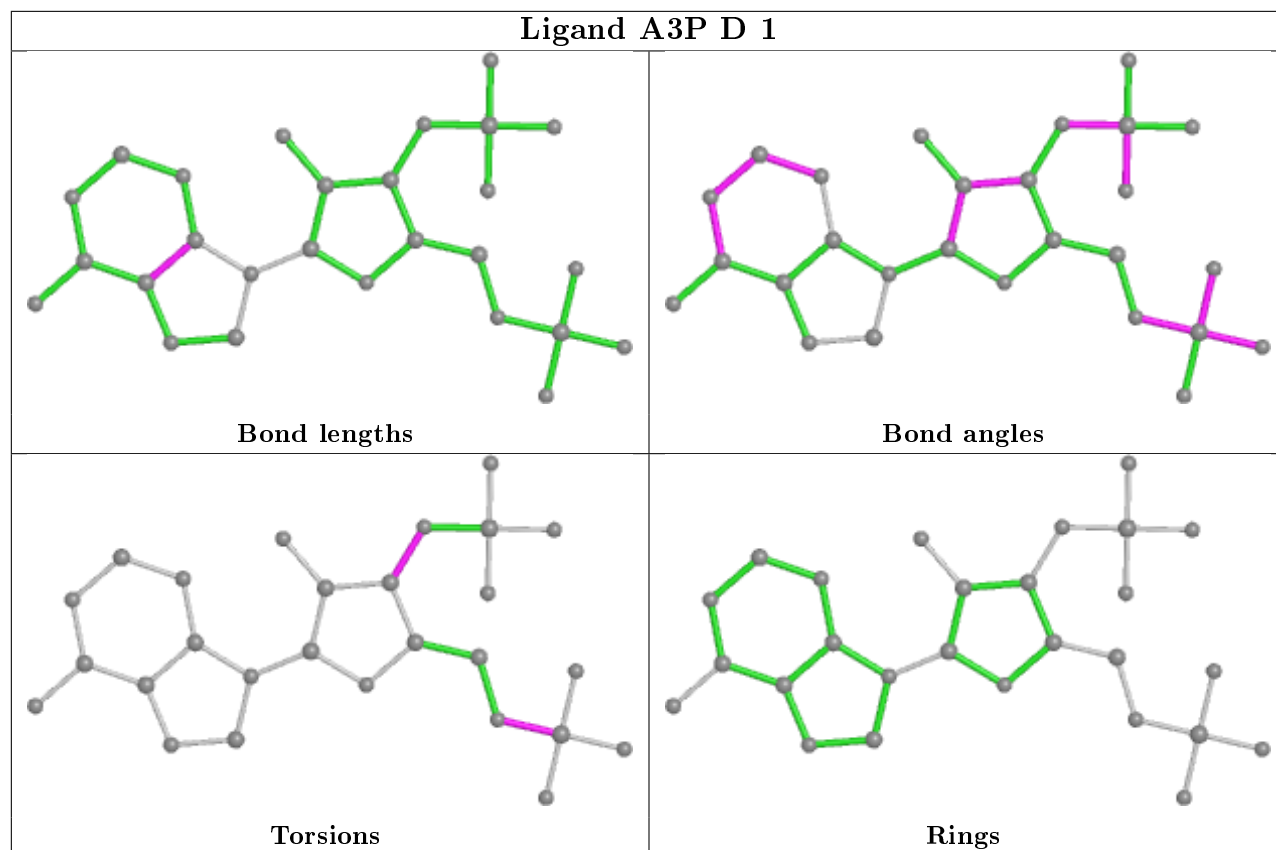
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	A3P	3	0
2	D	1	A3P	4	0
2	A	1	A3P	6	0
2	B	1	A3P	4	0

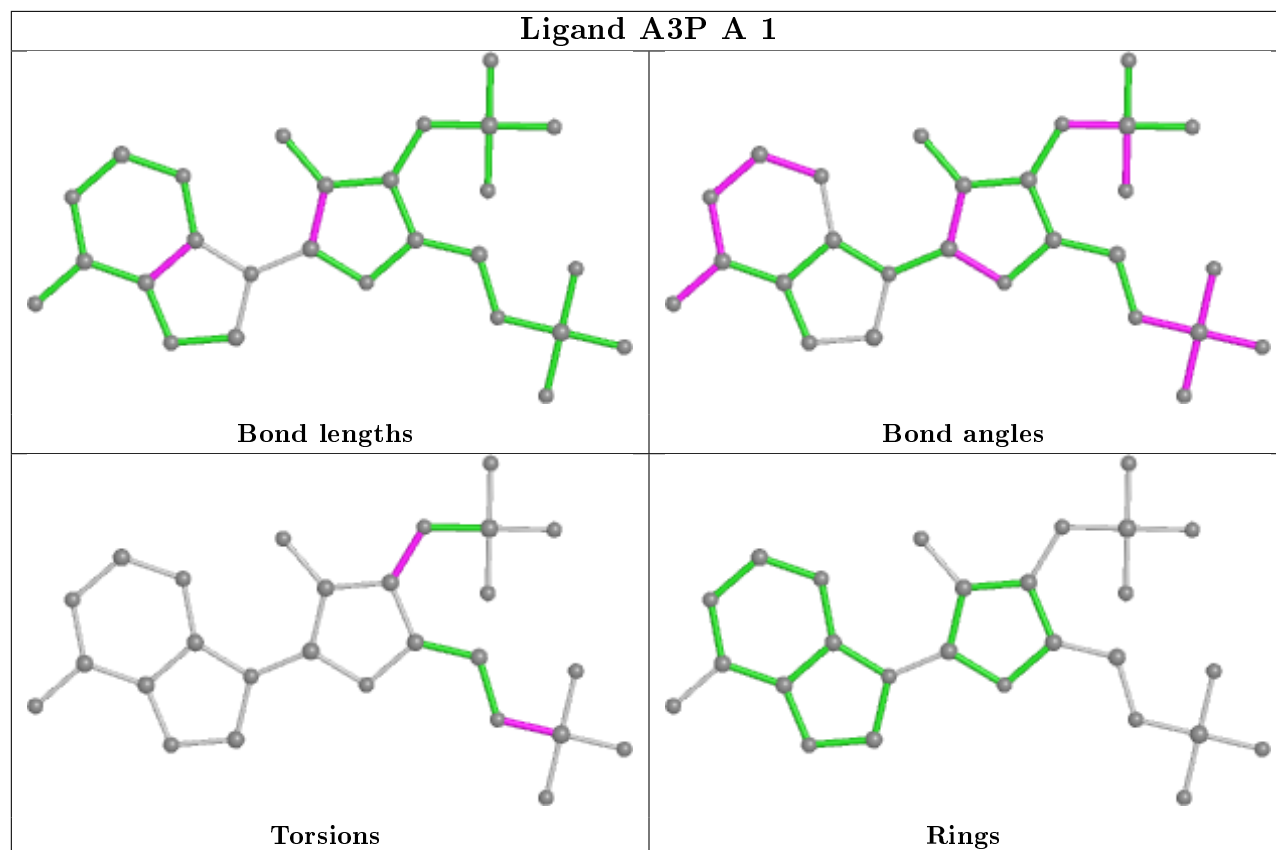
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

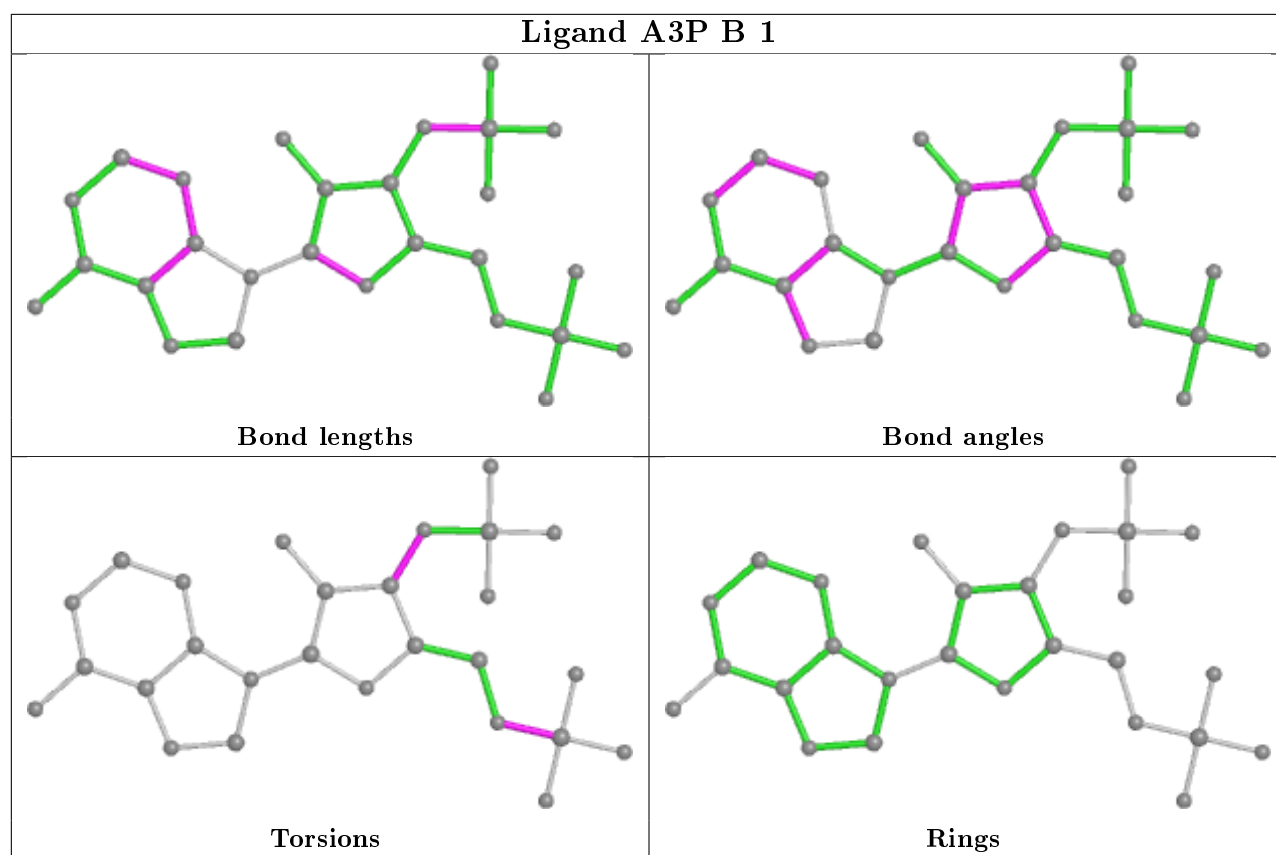


## Ligand A3P D 1



## Ligand A3P A 1





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	282/355 (79%)	0.19	9 (3%) 47 42	117, 124, 134, 146	0
1	B	285/355 (80%)	0.56	39 (13%) 3 4	118, 124, 134, 146	0
1	C	286/355 (80%)	0.09	8 (2%) 53 47	117, 124, 133, 146	0
1	D	292/355 (82%)	0.16	8 (2%) 54 48	117, 124, 133, 146	0
All	All	1145/1420 (80%)	0.25	64 (5%) 24 22	117, 124, 134, 146	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	ASP	7.2
1	B	182	VAL	5.9
1	B	278	SER	5.3
1	B	334	TYR	4.3
1	B	75	GLY	4.2
1	B	265	LEU	4.2
1	B	337	PRO	4.1
1	A	61	VAL	4.0
1	D	352	ASP	3.9
1	B	271	ILE	3.8
1	B	148	HIS	3.8
1	B	272	GLY	3.5
1	B	267	HIS	3.5
1	B	264	VAL	3.4
1	B	238	TYR	3.3
1	B	279	LEU	3.2
1	B	236	VAL	3.2
1	B	351	GLY	3.1
1	B	350	LYS	3.1
1	B	281	LYS	3.0
1	B	348	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	TYR	3.0
1	B	336	ASN	3.0
1	A	87	MET	2.8
1	A	127	GLY	2.8
1	B	340	PHE	2.8
1	B	291	LYS	2.7
1	A	126	ALA	2.7
1	C	247[A]	ARG	2.7
1	D	61	VAL	2.7
1	B	280	SER	2.7
1	D	179	LEU	2.7
1	B	317	ALA	2.7
1	D	130	ASP	2.5
1	D	343	ASN	2.5
1	A	114	SER	2.5
1	B	185	GLY	2.4
1	B	330	ASN	2.4
1	B	335	GLY	2.4
1	B	181	MET	2.4
1	D	243	LEU	2.3
1	A	63	ARG	2.3
1	B	277	VAL	2.2
1	B	274	PRO	2.2
1	B	339	PRO	2.2
1	B	283	GLU	2.2
1	A	258	ILE	2.2
1	B	344	ASN	2.2
1	C	126	ALA	2.2
1	B	293	VAL	2.2
1	B	347	ARG	2.2
1	C	346	GLN	2.2
1	B	289	VAL	2.1
1	B	87	MET	2.1
1	C	264	VAL	2.1
1	C	236	VAL	2.1
1	C	344	ASN	2.1
1	C	248	SER	2.1
1	B	205	SER	2.1
1	B	338	ASP	2.1
1	D	87	MET	2.1
1	A	152	ALA	2.0
1	C	316	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	350	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

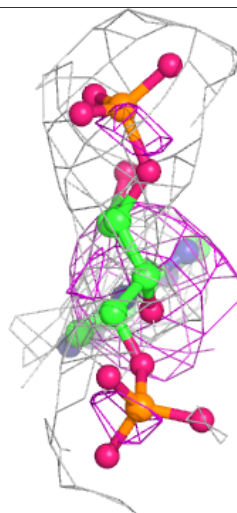
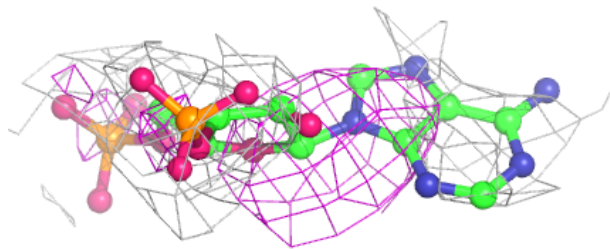
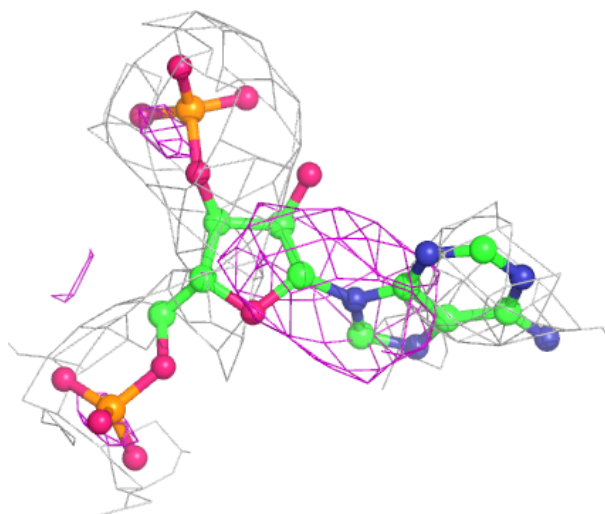
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A3P	B	1	27/27	0.72	0.46	114,117,119,120	0
2	A3P	C	1	27/27	0.92	0.19	65,68,72,73	0
2	A3P	D	1	27/27	0.93	0.20	53,63,69,70	0
2	A3P	A	1	27/27	0.95	0.19	46,53,55,56	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 A3P B 1:**

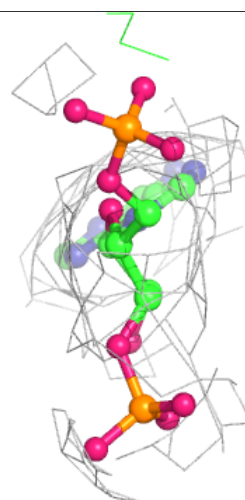
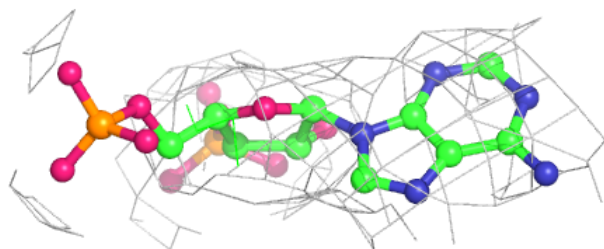
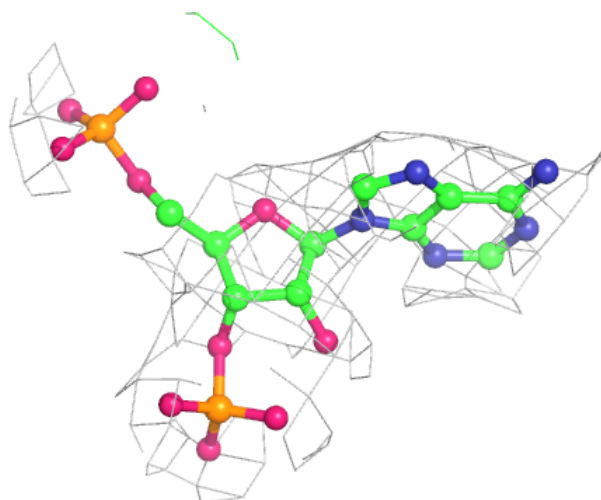
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





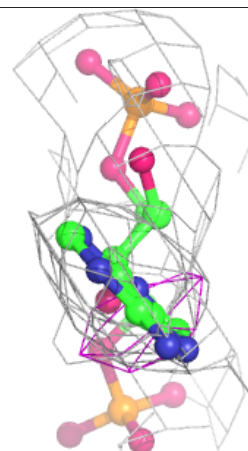
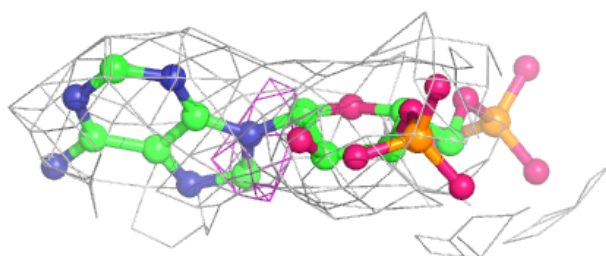
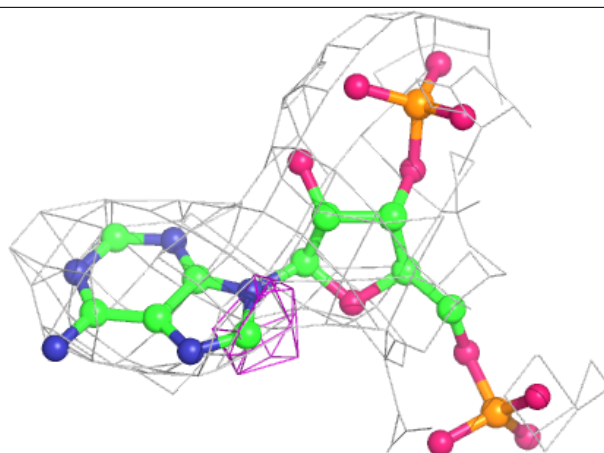
**Electron density around A3P C 1:**

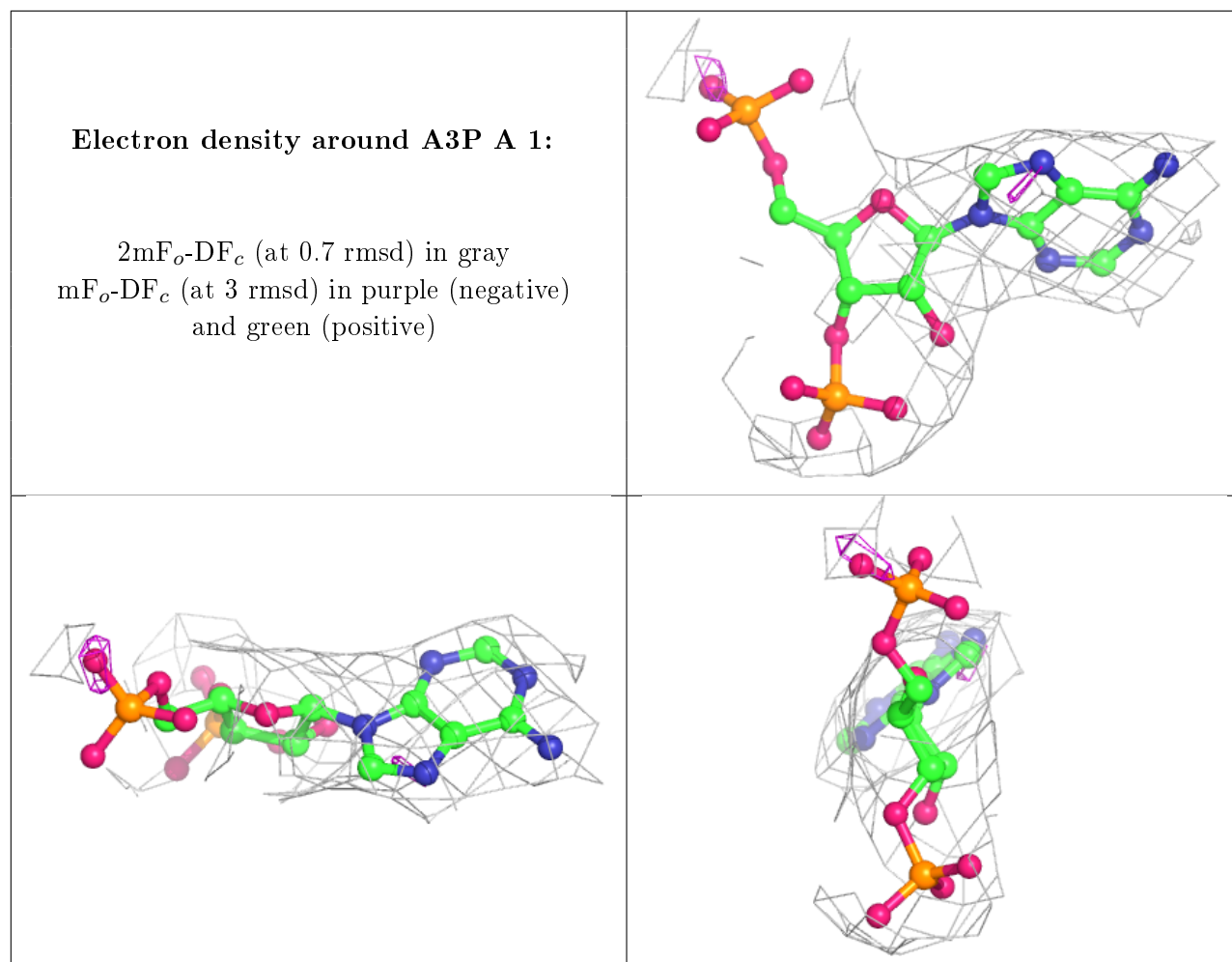
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A3P D 1:**

$2mF_o-DF_c$  (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.