



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:41 am BST

PDB ID : 3MGB
Title : Teg 12 Ternary Structure Complexed with PAP and the Teicoplanin Aglycone
Authors : Bick, M.J.; Banik, J.J.; Darst, S.A.; Brady, S.F.
Deposited on : 2010-04-05
Resolution : 2.04 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 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

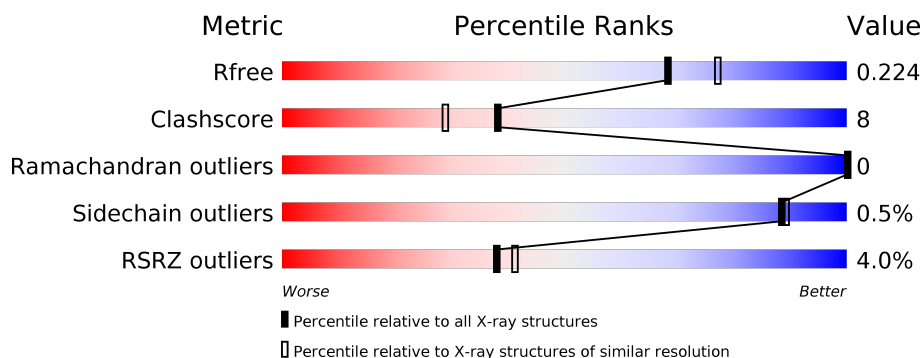
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 ≥ 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	319	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>10%</div> </div> </div>
1	B	319	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>17%</div> </div> </div>
2	C	7	<div> <div>14%</div> <div>71%</div> <div>14%</div> </div>
2	D	7	<div> <div>29%</div> <div>57%</div> <div>14%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4820 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 TEG12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2197	1378	392	416	11			
1	B	264	Total	C	N	O	S	0	0	0
			2050	1294	353	393	10			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	EXPRESSION TAG	UNP B7T1D7
A	-32	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	-31	SER	-	EXPRESSION TAG	UNP B7T1D7
A	-30	SER	-	EXPRESSION TAG	UNP B7T1D7
A	-29	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-28	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-27	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-26	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-25	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-24	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-23	SER	-	EXPRESSION TAG	UNP B7T1D7
A	-22	SER	-	EXPRESSION TAG	UNP B7T1D7
A	-21	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	-20	LEU	-	EXPRESSION TAG	UNP B7T1D7
A	-19	VAL	-	EXPRESSION TAG	UNP B7T1D7
A	-18	PRO	-	EXPRESSION TAG	UNP B7T1D7
A	-17	ARG	-	EXPRESSION TAG	UNP B7T1D7
A	-16	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	-15	SER	-	EXPRESSION TAG	UNP B7T1D7
A	-14	HIS	-	EXPRESSION TAG	UNP B7T1D7
A	-13	MET	-	EXPRESSION TAG	UNP B7T1D7
A	-12	ALA	-	EXPRESSION TAG	UNP B7T1D7
A	-11	SER	-	EXPRESSION TAG	UNP B7T1D7
A	-10	MET	-	EXPRESSION TAG	UNP B7T1D7
A	-9	THR	-	EXPRESSION TAG	UNP B7T1D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	-7	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	-6	GLN	-	EXPRESSION TAG	UNP B7T1D7
A	-5	GLN	-	EXPRESSION TAG	UNP B7T1D7
A	-4	MET	-	EXPRESSION TAG	UNP B7T1D7
A	-3	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	-2	ARG	-	EXPRESSION TAG	UNP B7T1D7
A	-1	GLY	-	EXPRESSION TAG	UNP B7T1D7
A	0	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-33	MET	-	EXPRESSION TAG	UNP B7T1D7
B	-32	GLY	-	EXPRESSION TAG	UNP B7T1D7
B	-31	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-30	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-29	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-28	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-27	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-26	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-25	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-24	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-23	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-22	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-21	GLY	-	EXPRESSION TAG	UNP B7T1D7
B	-20	LEU	-	EXPRESSION TAG	UNP B7T1D7
B	-19	VAL	-	EXPRESSION TAG	UNP B7T1D7
B	-18	PRO	-	EXPRESSION TAG	UNP B7T1D7
B	-17	ARG	-	EXPRESSION TAG	UNP B7T1D7
B	-16	GLY	-	EXPRESSION TAG	UNP B7T1D7
B	-15	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-14	HIS	-	EXPRESSION TAG	UNP B7T1D7
B	-13	MET	-	EXPRESSION TAG	UNP B7T1D7
B	-12	ALA	-	EXPRESSION TAG	UNP B7T1D7
B	-11	SER	-	EXPRESSION TAG	UNP B7T1D7
B	-10	MET	-	EXPRESSION TAG	UNP B7T1D7
B	-9	THR	-	EXPRESSION TAG	UNP B7T1D7
B	-8	GLY	-	EXPRESSION TAG	UNP B7T1D7
B	-7	GLY	-	EXPRESSION TAG	UNP B7T1D7
B	-6	GLN	-	EXPRESSION TAG	UNP B7T1D7
B	-5	GLN	-	EXPRESSION TAG	UNP B7T1D7
B	-4	MET	-	EXPRESSION TAG	UNP B7T1D7
B	-3	GLY	-	EXPRESSION TAG	UNP B7T1D7
B	-2	ARG	-	EXPRESSION TAG	UNP B7T1D7
B	-1	GLY	-	EXPRESSION TAG	UNP B7T1D7

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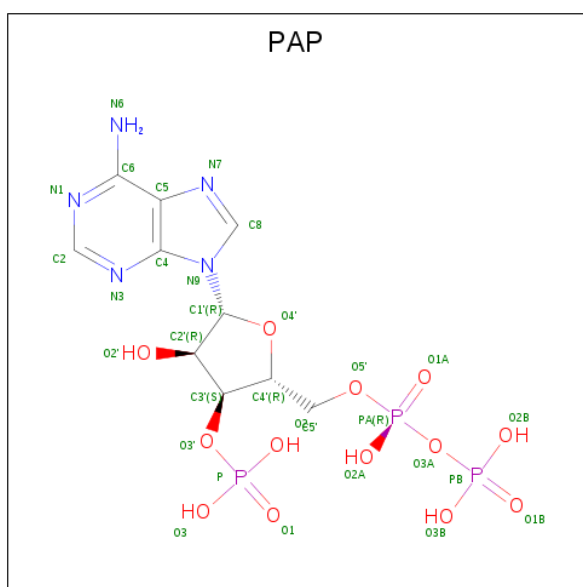
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	EXPRESSION TAG	UNP B7T1D7

- Molecule 2 is a protein called TEICOPLANIN AGLYCON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	Cl	N	O	0	0	0
			85	58	2	7	18			
2	D	7	Total	C	Cl	N	O	2	0	0
			85	58	2	7	18			

- Molecule 3 is 3'-PHOSPHATE-ADENOSINE-5'-DIPHOSPHATE (three-letter code: PAP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

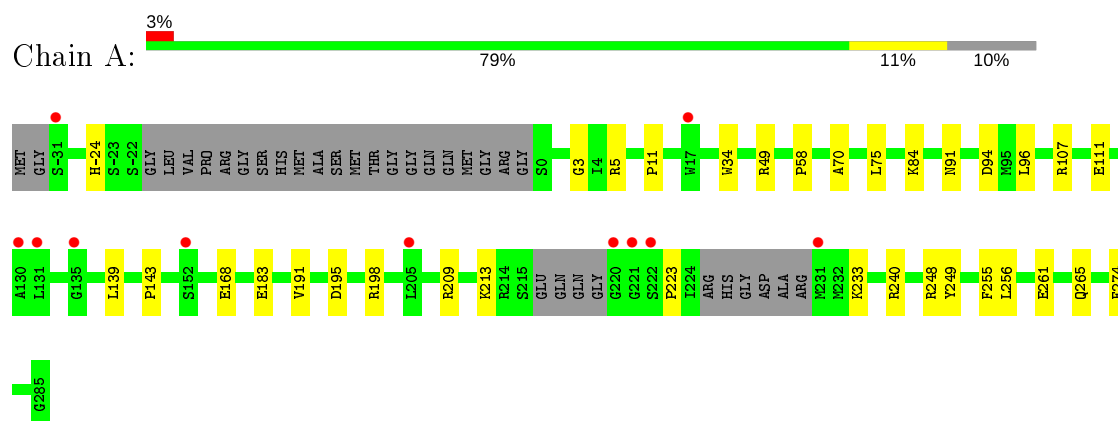
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		
6	B	131	Total	O	0	0
			131	131		
6	C	9	Total	O	0	0
			9	9		
6	D	10	Total	O	0	0
			10	10		

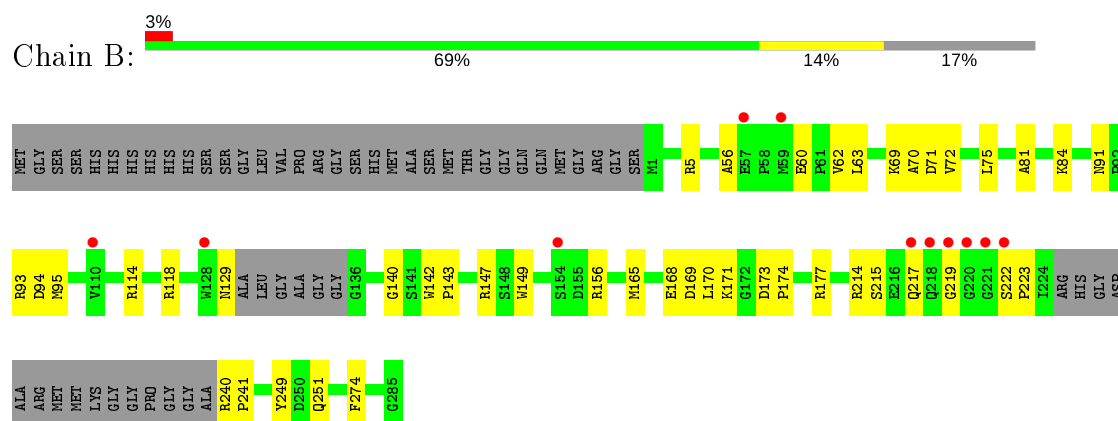
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

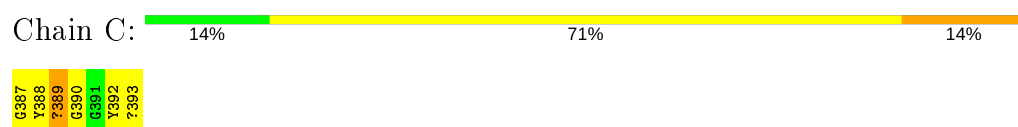
• Molecule 1: TEG12



• Molecule 1: TEG12



• Molecule 2: TEICOPLANIN AGLYCON



• Molecule 2: TEICOPLANIN AGLYCON



G387
Y388
Y389
G390
G391
Y392
Y393

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.00Å 78.34Å 99.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.95 – 2.04 36.32 – 2.04	Depositor EDS
% Data completeness (in resolution range)	93.1 (32.95-2.04) 97.2 (36.32-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.05Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.171 , 0.225 0.172 , 0.224	Depositor DCC
R_{free} test set	1941 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4820	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: PAP, GHP, 3MY, CL, ACT, 3FG, OMY

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	0.38	0/2247	0.53	0/3035
1	B	0.36	0/2094	0.52	0/2835
All	All	0.37	0/4341	0.53	0/5870

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	389	3FG	Mainchain
2	D	391	GHP	Mainchain

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	2197	0	2112	26	0
1	B	2050	0	1972	31	0
2	C	85	0	40	6	0
2	D	85	0	40	6	0
3	A	27	0	11	0	0
3	B	27	0	11	0	0
4	A	8	0	6	0	0
5	A	1	0	0	0	0
6	A	190	0	0	3	0
6	B	131	0	0	3	0
6	C	9	0	0	0	0
6	D	10	0	0	0	0
All	All	4820	0	4192	66	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 8.

All (66) 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:114:ARG:HH21	1:B:118:ARG:HH21	1.19	0.91
1:A:168:GLU:HG2	1:A:249:TYR:CE1	2.22	0.75
1:B:114:ARG:NH2	1:B:118:ARG:HH21	1.89	0.71
1:B:114:ARG:HH21	1:B:118:ARG:NH2	1.92	0.67
1:B:5:ARG:HB2	1:B:63:LEU:HD23	1.80	0.63
1:A:183:GLU:HG3	1:A:191:VAL:HG21	1.81	0.63
1:B:143:PRO:HG3	1:B:274:PHE:HA	1.83	0.60
1:A:70:ALA:HA	1:A:75:LEU:HD23	1.83	0.60
1:A:168:GLU:HG2	1:A:249:TYR:CD1	2.38	0.59
1:A:34:TRP:CE2	1:A:223:PRO:HG3	2.39	0.58
1:A:107:ARG:HD3	1:A:255:PHE:CE1	2.39	0.57
1:A:143:PRO:HG3	1:A:274:PHE:HA	1.86	0.57
1:A:3:GLY:HA2	1:A:58:PRO:HG2	1.86	0.57
1:B:56:ALA:O	1:B:81:ALA:HB2	2.05	0.56
1:A:195:ASP:HA	1:A:198:ARG:NH1	2.21	0.56
1:A:34:TRP:CZ2	1:A:223:PRO:HG3	2.41	0.55
1:B:71:ASP:HB3	1:B:156:ARG:HE	1.71	0.54
1:A:5:ARG:HG3	1:A:84:LYS:HB2	1.90	0.54
1:A:195:ASP:HA	1:A:198:ARG:HH11	1.73	0.53
1:B:5:ARG:HG3	1:B:84:LYS:HB2	1.89	0.53
1:A:111:GLU:HG3	6:A:2079:HOH:O	2.09	0.53
1:B:174:PRO:HD2	6:B:2080:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:MET:SD	1:B:177:ARG:HB3	2.50	0.51
1:A:70:ALA:HA	1:A:75:LEU:CD2	2.40	0.51
2:D:391:GHP:H6	2:D:392:OMY:C	2.41	0.51
1:B:95:MET:HE1	1:B:142:TRP:CD1	2.46	0.50
1:B:142:TRP:HB3	1:B:143:PRO:HD3	1.93	0.50
1:A:91:ASN:HB3	1:A:94:ASP:OD2	2.11	0.50
2:D:391:GHP:C6	2:D:393:3FG:N	2.75	0.50
1:A:240:ARG:O	2:C:388:3MY:HB2C	2.13	0.48
1:A:248:ARG:NH2	6:A:2160:HOH:O	2.46	0.48
1:B:214:ARG:HA	1:B:217:GLN:OE1	2.13	0.48
1:A:261:GLU:O	1:A:265:GLN:HG2	2.14	0.47
1:A:96:LEU:HD23	1:A:96:LEU:C	2.35	0.47
1:B:69:LYS:HD3	1:B:140:GLY:HA3	1.96	0.47
1:B:93:ARG:HD3	1:B:251:GLN:O	2.15	0.47
1:A:183:GLU:CG	1:A:191:VAL:HG21	2.43	0.47
1:B:72:VAL:HG22	1:B:75:LEU:HD23	1.97	0.46
2:D:390:GHP:H6	2:D:392:OMY:CE1	2.45	0.46
2:C:387:GHP:C2	2:C:389:3FG:HG2	2.46	0.46
1:A:209:ARG:O	1:A:213:LYS:HG3	2.15	0.45
1:A:195:ASP:OD2	1:A:198:ARG:NH1	2.49	0.45
1:A:11:PRO:HG2	1:A:139:LEU:HD21	1.98	0.45
1:B:72:VAL:CG2	1:B:75:LEU:HD23	2.47	0.45
1:B:70:ALA:HB2	1:B:149:TRP:CD2	2.52	0.45
2:C:392:OMY:HD2	2:D:390:GHP:N	2.33	0.44
2:C:390:GHP:H6	2:C:392:OMY:CE1	2.47	0.44
2:C:387:GHP:C2	2:C:389:3FG:CG2	2.96	0.43
1:A:-24:HIS:HA	2:C:393:3FG:C	2.48	0.43
1:B:129:ASN:ND2	6:B:2057:HOH:O	2.45	0.43
2:D:389:3FG:HA	2:D:390:GHP:HA	1.83	0.43
1:B:143:PRO:HG3	1:B:274:PHE:CA	2.47	0.43
1:B:168:GLU:HG2	1:B:249:TYR:CD1	2.54	0.43
1:A:233:LYS:HA	1:A:233:LYS:HD2	1.85	0.43
1:B:240:ARG:HA	1:B:241:PRO:HD3	1.91	0.43
1:B:71:ASP:HB3	1:B:156:ARG:NE	2.33	0.42
1:B:170:LEU:HD23	1:B:177:ARG:HB2	2.01	0.42
1:B:222:SER:OG	1:B:223:PRO:HD2	2.19	0.42
2:D:391:GHP:C6	2:D:392:OMY:C	2.98	0.42
1:B:169:ASP:O	1:B:177:ARG:HG3	2.20	0.42
1:B:147:ARG:HD2	6:B:2062:HOH:O	2.19	0.42
1:A:49:ARG:NH1	6:A:2039:HOH:O	2.53	0.42
1:B:215:SER:O	1:B:219:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:HB3	1:B:94:ASP:OD2	2.21	0.41
1:B:173:ASP:O	1:B:177:ARG:HG2	2.21	0.40
1:B:60:GLU:O	1:B:62:VAL:HG23	2.21	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	278/319 (87%)	272 (98%)	6 (2%)	0	100	100
1	B	258/319 (81%)	253 (98%)	5 (2%)	0	100	100
All	All	536/638 (84%)	525 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	225/253 (89%)	224 (100%)	1 (0%)	91	91
1	B	211/253 (83%)	210 (100%)	1 (0%)	88	89
All	All	436/506 (86%)	434 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	LEU
1	B	171	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	269	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3MY	D	388	2	12,13,14	1.61	3 (25%)	14,17,19	1.89	2 (14%)
2	GHP	D	387	2	10,11,12	3.52	6 (60%)	11,14,16	1.11	1 (9%)
2	3FG	C	393	2	9,13,13	5.17	5 (55%)	13,18,18	0.79	1 (7%)
2	3FG	C	389	2	11,12,13	4.18	6 (54%)	13,16,18	0.83	0
2	GHP	C	387	2	10,11,12	3.78	6 (60%)	11,14,16	1.09	2 (18%)
2	OMY	D	392	2	12,14,15	2.81	4 (33%)	17,19,21	2.68	6 (35%)
2	GHP	C	391	2	10,11,12	4.44	7 (70%)	11,14,16	1.70	3 (27%)
2	3FG	D	393	2	9,13,13	5.19	5 (55%)	13,18,18	0.74	0
2	3MY	C	388	2	12,13,14	1.61	3 (25%)	14,17,19	1.01	0
2	OMY	C	392	2	12,14,15	2.70	4 (33%)	17,19,21	2.32	6 (35%)
2	GHP	D	391	2	10,11,12	4.31	6 (60%)	11,14,16	1.49	3 (27%)
2	3FG	D	389	2	11,12,13	4.02	6 (54%)	13,16,18	0.84	0
2	GHP	C	390	2	10,11,12	4.60	6 (60%)	11,14,16	1.91	4 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GHP	D	390	2	10,11,12	4.43	6 (60%)	11,14,16	1.68	3 (27%)

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	3MY	D	388	2	-	2/5/6/8	0/1/1/1
2	GHP	D	387	2	-	2/4/6/8	0/1/1/1
2	3FG	C	393	2	-	2/4/8/8	0/1/1/1
2	3FG	C	389	2	-	0/4/6/8	0/1/1/1
2	GHP	C	387	2	-	4/4/6/8	0/1/1/1
2	OMY	D	392	2	-	0/9/10/12	0/1/1/1
2	GHP	C	391	2	-	0/4/6/8	0/1/1/1
2	3FG	D	393	2	-	1/4/8/8	0/1/1/1
2	3MY	C	388	2	-	0/5/6/8	0/1/1/1
2	OMY	C	392	2	-	1/9/10/12	0/1/1/1
2	GHP	D	391	2	-	0/4/6/8	0/1/1/1
2	3FG	D	389	2	-	0/4/6/8	0/1/1/1
2	GHP	C	390	2	-	2/4/6/8	0/1/1/1
2	GHP	D	390	2	-	2/4/6/8	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	393	3FG	CG1-CB	9.85	1.54	1.39
2	C	393	3FG	CG1-CB	9.82	1.54	1.39
2	C	389	3FG	CG2-CB	8.42	1.52	1.39
2	D	389	3FG	CG2-CB	8.14	1.51	1.39
2	D	393	3FG	CZ-CD1	7.63	1.50	1.39
2	C	393	3FG	CZ-CD1	7.52	1.50	1.39
2	D	391	GHP	C6-C1	7.39	1.51	1.39
2	C	391	GHP	C6-C1	7.31	1.50	1.39
2	D	392	OMY	CZ-CE1	7.20	1.46	1.39
2	D	393	3FG	CZ-CD2	7.12	1.49	1.39
2	C	390	GHP	C6-C1	7.11	1.50	1.39
2	D	390	GHP	C6-C1	7.02	1.50	1.39
2	C	393	3FG	CZ-CD2	6.98	1.49	1.39
2	C	392	OMY	CZ-CE1	6.88	1.46	1.39
2	D	390	GHP	C6-C5	6.35	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	390	GHP	C6-C5	6.30	1.50	1.38
2	C	389	3FG	CZ-CD1	6.18	1.48	1.39
2	C	391	GHP	C5-C4	6.07	1.50	1.38
2	D	389	3FG	CZ-CD1	6.00	1.48	1.39
2	D	391	GHP	C3-C2	5.96	1.49	1.38
2	C	391	GHP	C3-C2	5.93	1.49	1.38
2	C	389	3FG	CG1-CD1	5.78	1.47	1.39
2	C	390	GHP	C3-C4	5.78	1.49	1.38
2	C	390	GHP	C3-C2	5.74	1.49	1.38
2	D	390	GHP	C2-C1	5.67	1.48	1.39
2	D	389	3FG	CG1-CD1	5.65	1.47	1.39
2	D	390	GHP	C3-C2	5.57	1.48	1.38
2	D	391	GHP	C5-C4	5.43	1.49	1.38
2	D	391	GHP	C3-C4	5.43	1.49	1.38
2	C	387	GHP	C6-C1	5.27	1.47	1.39
2	C	389	3FG	CZ-CD2	5.27	1.47	1.39
2	C	390	GHP	C2-C1	5.26	1.47	1.39
2	C	391	GHP	C2-C1	5.21	1.47	1.39
2	C	387	GHP	C2-C1	5.18	1.47	1.39
2	C	393	3FG	CG2-CD2	5.17	1.46	1.39
2	D	387	GHP	C6-C1	5.05	1.47	1.39
2	C	391	GHP	C3-C4	5.02	1.48	1.38
2	C	387	GHP	C3-C2	4.97	1.47	1.38
2	D	393	3FG	CG2-CD2	4.97	1.46	1.39
2	D	391	GHP	C2-C1	4.97	1.47	1.39
2	C	390	GHP	C5-C4	4.88	1.48	1.38
2	D	387	GHP	C2-C1	4.85	1.46	1.39
2	D	389	3FG	CZ-CD2	4.84	1.46	1.39
2	D	390	GHP	C3-C4	4.63	1.47	1.38
2	C	387	GHP	C6-C5	4.60	1.47	1.38
2	D	387	GHP	C3-C2	4.58	1.47	1.38
2	C	387	GHP	C5-C4	4.53	1.47	1.38
2	D	390	GHP	C5-C4	4.49	1.47	1.38
2	D	387	GHP	C6-C5	4.49	1.46	1.38
2	C	387	GHP	C3-C4	4.37	1.47	1.38
2	D	387	GHP	C5-C4	4.25	1.47	1.38
2	C	392	OMY	CD2-CG	4.24	1.45	1.39
2	D	392	OMY	CD2-CG	3.82	1.45	1.39
2	D	387	GHP	C3-C4	3.80	1.46	1.38
2	D	392	OMY	CD1-CG	3.73	1.44	1.39
2	C	391	GHP	C6-C5	3.65	1.45	1.38
2	C	393	3FG	CG2-CB	3.04	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	388	3MY	CZ-CE2	3.03	1.42	1.39
2	D	393	3FG	CG2-CB	3.01	1.43	1.39
2	C	389	3FG	CG2-CD2	2.90	1.43	1.39
2	D	389	3FG	CG2-CD2	2.89	1.43	1.39
2	C	392	OMY	CD1-CG	2.70	1.43	1.39
2	D	391	GHP	C6-C5	2.69	1.43	1.38
2	D	388	3MY	CD2-CG	2.68	1.43	1.39
2	D	388	3MY	CZ-CE2	2.67	1.42	1.39
2	D	388	3MY	CE1-CZ	2.52	1.44	1.39
2	C	389	3FG	CG1-CB	2.52	1.43	1.39
2	C	388	3MY	CD2-CG	2.36	1.43	1.39
2	D	389	3FG	CG1-CB	2.29	1.42	1.39
2	C	388	3MY	CE1-CZ	2.25	1.43	1.39
2	C	391	GHP	C1-CA	-2.21	1.50	1.52
2	C	392	OMY	CE2-CZ	2.08	1.43	1.39
2	D	392	OMY	ODE-CB	-2.01	1.38	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	392	OMY	CG-CB-CA	-6.63	102.62	111.49
2	D	392	OMY	CD1-CE1-CZ	-6.32	117.25	120.91
2	D	388	3MY	CD2-CE2-CZ	-5.01	118.01	120.91
2	D	392	OMY	CE2-CZ-CE1	4.91	123.31	118.55
2	D	392	OMY	CG-CB-CA	-4.29	105.74	111.49
2	C	390	GHP	C6-C1-C2	3.68	122.89	118.29
2	D	390	GHP	C5-C6-C1	-3.56	117.61	121.20
2	C	392	OMY	CE2-CZ-CE1	3.49	121.94	118.55
2	D	388	3MY	CE1-CZ-CE2	3.42	121.87	118.55
2	C	391	GHP	C5-C6-C1	-3.29	117.88	121.20
2	C	392	OMY	ODE-CB-CA	3.25	114.13	107.28
2	C	390	GHP	C5-C6-C1	-3.20	117.98	121.20
2	C	391	GHP	C6-C1-C2	3.17	122.25	118.29
2	D	392	OMY	CD2-CG-CD1	3.06	122.28	118.76
2	D	392	OMY	CD2-CG-CB	-2.94	116.35	120.73
2	C	390	GHP	C3-C2-C1	-2.91	118.27	121.20
2	D	390	GHP	C6-C1-C2	2.70	121.66	118.29
2	D	391	GHP	C6-C1-C2	2.69	121.65	118.29
2	D	391	GHP	C3-C2-C1	-2.68	118.50	121.20
2	D	392	OMY	CE2-CD2-CG	-2.62	118.56	121.20
2	C	392	OMY	CD1-CE1-CZ	-2.40	119.52	120.91
2	C	390	GHP	C2-C1-CA	-2.36	116.86	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	392	OMY	CD2-CG-CD1	2.32	121.44	118.76
2	D	391	GHP	C6-C1-CA	-2.20	117.10	120.65
2	D	387	GHP	C3-C2-C1	-2.20	118.99	121.20
2	C	392	OMY	CD2-CE2-CZ	-2.19	118.25	120.50
2	C	387	GHP	C6-C1-C2	2.17	121.00	118.29
2	D	390	GHP	C3-C2-C1	-2.17	119.02	121.20
2	C	387	GHP	C3-C2-C1	-2.05	119.14	121.20
2	C	391	GHP	C3-C2-C1	-2.03	119.15	121.20
2	C	393	3FG	C-CA-CB	2.00	113.87	111.28

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	388	3MY	C-CA-CB-CG
2	D	388	3MY	N-CA-CB-CG
2	C	392	OMY	O-C-CA-CB
2	C	387	GHP	C6-C1-CA-C
2	C	393	3FG	C-CA-CB-CG1
2	C	393	3FG	C-CA-CB-CG2
2	D	393	3FG	C-CA-CB-CG2
2	D	387	GHP	C6-C1-CA-C
2	C	387	GHP	C2-C1-CA-C
2	C	390	GHP	C2-C1-CA-C
2	C	390	GHP	C6-C1-CA-C
2	D	390	GHP	C2-C1-CA-C
2	D	390	GHP	C6-C1-CA-C
2	D	387	GHP	C2-C1-CA-N
2	C	387	GHP	C2-C1-CA-N
2	C	387	GHP	C6-C1-CA-N

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	393	3FG	1	0
2	C	389	3FG	2	0
2	C	387	GHP	2	0
2	D	392	OMY	3	0
2	D	393	3FG	1	0
2	C	388	3MY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	392	OMY	2	0
2	D	391	GHP	3	0
2	D	389	3FG	1	0
2	C	390	GHP	1	0
2	D	390	GHP	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	ACT	A	287	-	1,3,3	1.39	0	0,3,3	0.00	-
4	ACT	A	288	-	1,3,3	1.44	0	0,3,3	0.00	-
3	PAP	A	286	-	26,29,33	1.04	2 (7%)	31,45,52	1.43	4 (12%)
3	PAP	B	286	-	26,29,33	1.05	1 (3%)	31,45,52	1.45	5 (16%)

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	PAP	A	286	-	-	4/11/31/37	0/3/3/3
3	PAP	B	286	-	-	3/11/31/37	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	286	PAP	C5-C4	2.66	1.48	1.40
3	A	286	PAP	P-O3'	2.34	1.63	1.59
3	A	286	PAP	C2-N3	2.14	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	286	PAP	N3-C2-N1	-3.82	122.72	128.68
3	B	286	PAP	O3A-PA-O5'	-3.24	98.12	106.73
3	B	286	PAP	N3-C2-N1	-2.84	124.23	128.68
3	B	286	PAP	O2A-PA-O1A	2.58	120.78	110.68
3	B	286	PAP	C4-C5-N7	-2.55	106.74	109.40
3	A	286	PAP	C2-N1-C6	2.52	123.06	118.75
3	A	286	PAP	O4'-C1'-C2'	-2.44	103.36	106.93
3	B	286	PAP	O4'-C1'-C2'	-2.33	103.52	106.93
3	A	286	PAP	C2'-C3'-C4'	-2.03	99.62	103.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

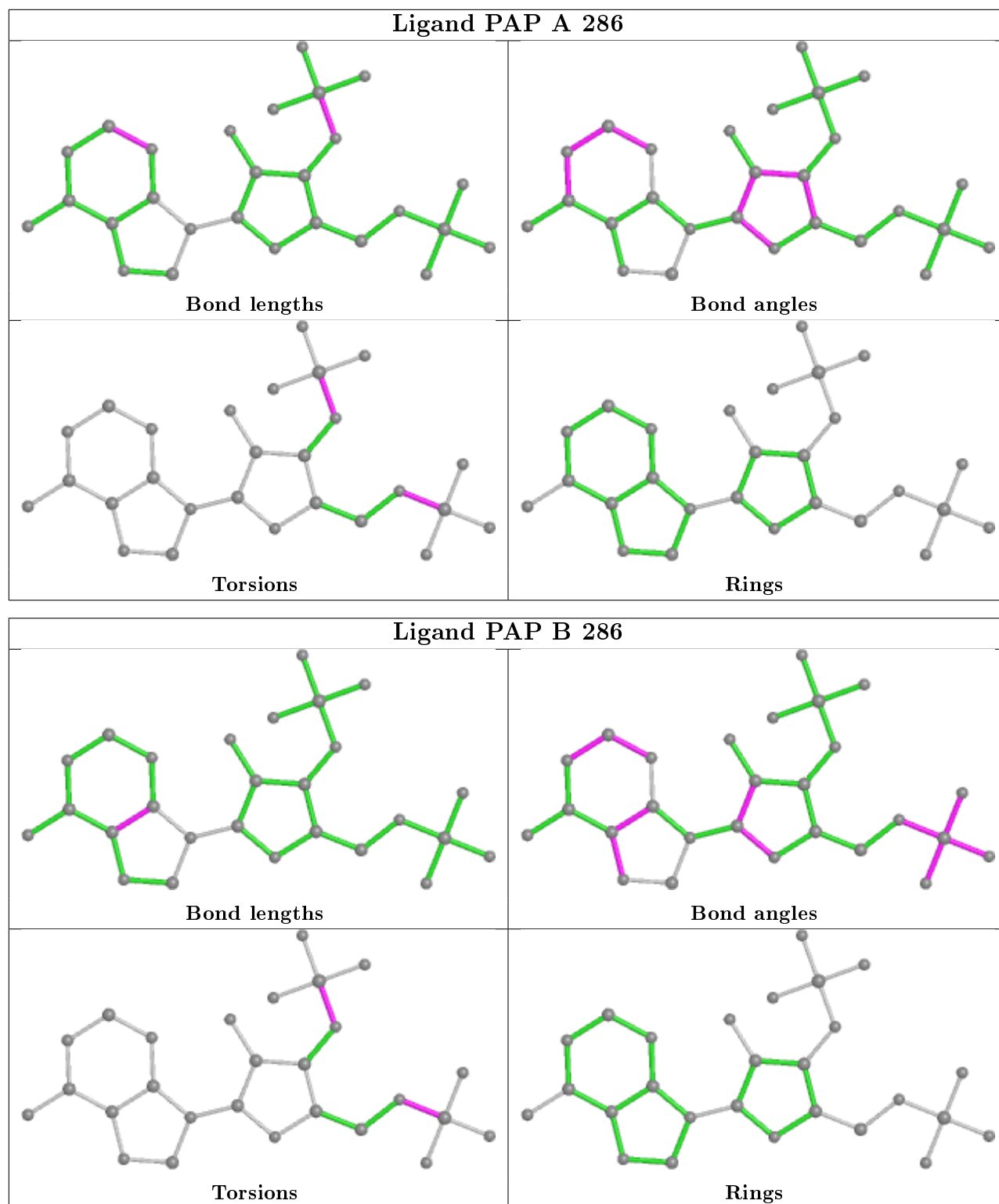
Mol	Chain	Res	Type	Atoms
3	A	286	PAP	C3'-O3'-P-O1
3	A	286	PAP	C3'-O3'-P-O2
3	B	286	PAP	C5'-O5'-PA-O2A
3	B	286	PAP	C5'-O5'-PA-O3A
3	B	286	PAP	C3'-O3'-P-O1
3	A	286	PAP	C5'-O5'-PA-O2A
3	A	286	PAP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	286/319 (89%)	-0.19	11 (3%) 40 44	14, 28, 69, 104	0
1	B	264/319 (82%)	-0.11	11 (4%) 36 39	19, 34, 80, 134	0
2	C	0/7	-	-	-	-
2	D	0/7	-	-	-	-
All	All	550/652 (84%)	-0.15	22 (4%) 38 41	14, 31, 72, 134	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	GLY	6.6
1	B	220	GLY	6.0
1	B	59	MET	4.9
1	A	231	MET	4.2
1	B	222	SER	4.2
1	A	131	LEU	4.0
1	A	221	GLY	3.5
1	A	130	ALA	3.3
1	B	221	GLY	3.1
1	A	222	SER	3.1
1	B	154	SER	3.0
1	B	128	TRP	2.6
1	B	110	VAL	2.6
1	B	217	GLN	2.5
1	A	-31	SER	2.5
1	A	220	GLY	2.4
1	A	205	LEU	2.3
1	A	17	TRP	2.2
1	B	57	GLU	2.2
1	A	152	SER	2.2
1	B	218	GLN	2.1
1	A	135	GLY	2.1

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
2	GHP	D	390	11/12	0.90	0.11	21,22,24,24	0
2	OMY	D	392	14/15	0.91	0.11	22,25,29,68	1
2	OMY	C	392	14/15	0.93	0.09	22,24,26,66	0
2	GHP	C	387	11/12	0.93	0.09	32,33,37,37	0
2	3MY	D	388	13/14	0.94	0.09	24,26,29,66	1
2	GHP	D	387	11/12	0.95	0.12	24,29,35,40	0
2	3FG	C	393	13/13	0.95	0.10	27,30,34,36	0
2	3FG	D	393	13/13	0.96	0.14	29,33,38,40	0
2	3MY	C	388	13/14	0.96	0.09	25,27,32,60	0
2	3FG	C	389	12/13	0.97	0.09	24,29,35,38	0
2	GHP	D	391	11/12	0.97	0.09	22,24,26,26	0
2	3FG	D	389	12/13	0.97	0.11	22,24,26,26	0
2	GHP	C	391	11/12	0.97	0.09	22,26,28,32	0
2	GHP	C	390	11/12	0.98	0.07	23,23,25,27	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

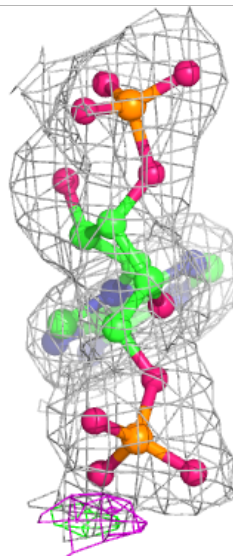
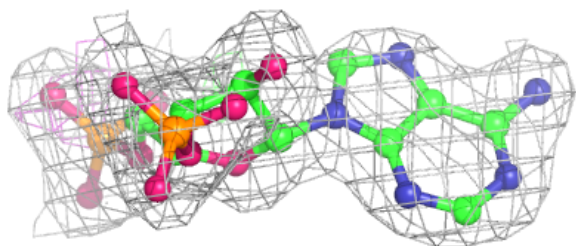
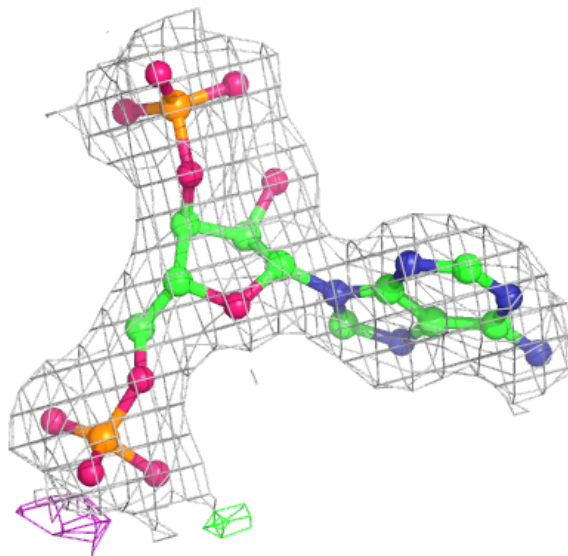
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	A	288	4/4	0.84	0.13	59,60,61,62	0
4	ACT	A	287	4/4	0.86	0.16	69,70,70,72	0
5	CL	A	289	1/1	0.89	0.11	65,65,65,65	0
3	PAP	B	286	27/31	0.97	0.11	27,35,39,39	0
3	PAP	A	286	27/31	0.99	0.19	16,20,22,23	0

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.

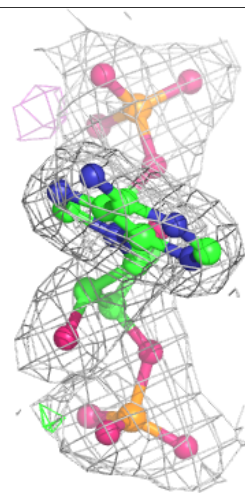
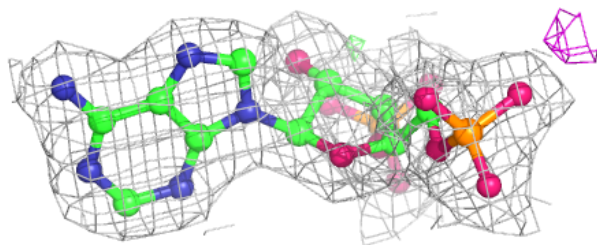
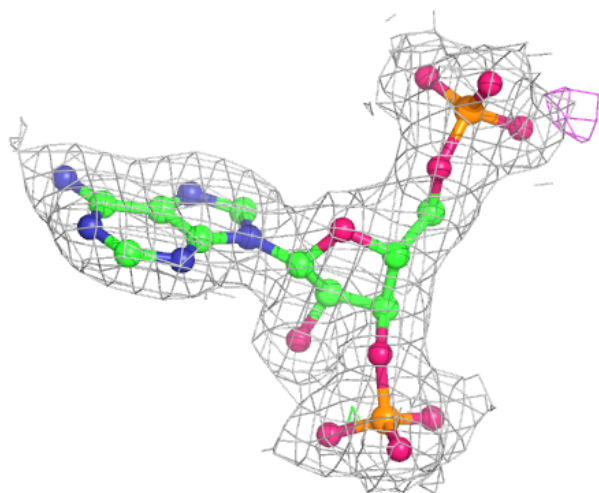
Electron density around PAP B 286:

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



Electron density around PAP A 286:

$2mF_o-DF_c$ (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.