



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:44 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

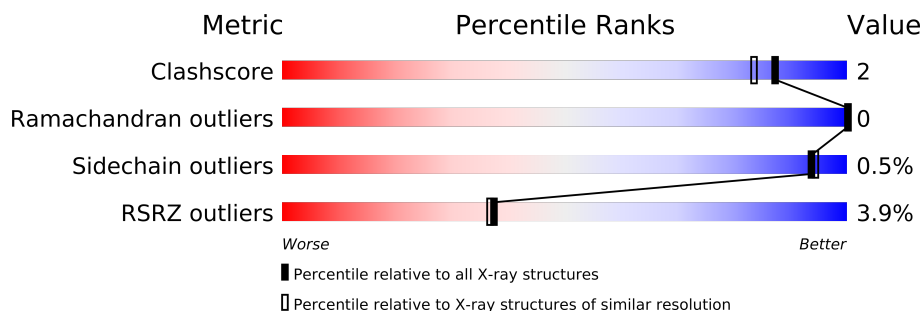
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	
2	C	7	
2	D	7	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ACT	A	287	-	X
4	ACT	A	288	-	X
5	CL	A	289	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4820 atoms, of which 0 are hydrogen and 0 are deuterium.

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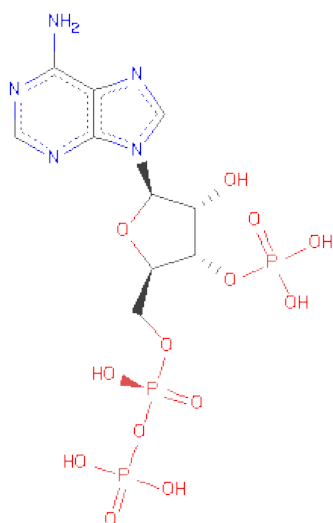
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	EXPRESSION TAG	UNP B7T1D7

- Molecule 2 is a protein called TEICOPLANIN AGLYCONE.

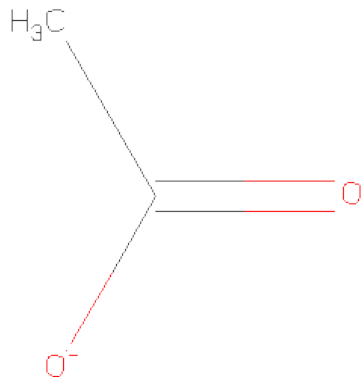
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total 85	C 58	Cl 2	N 7	O 18	0	0	0
2	D	7	Total 85	C 58	Cl 2	N 7	O 18	2	0	0

- 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 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- 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		

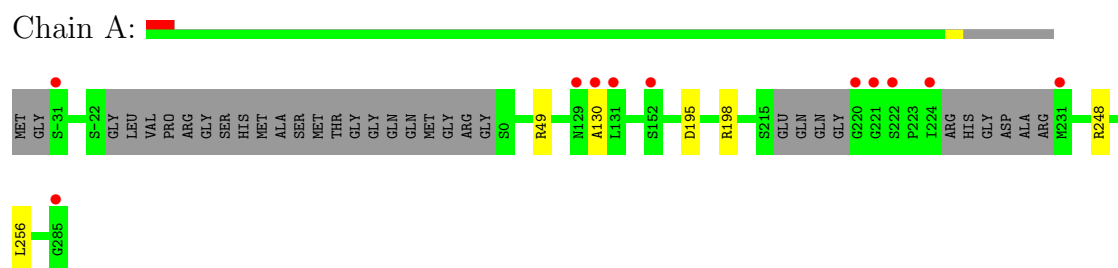
- Molecule 6 is water.

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		

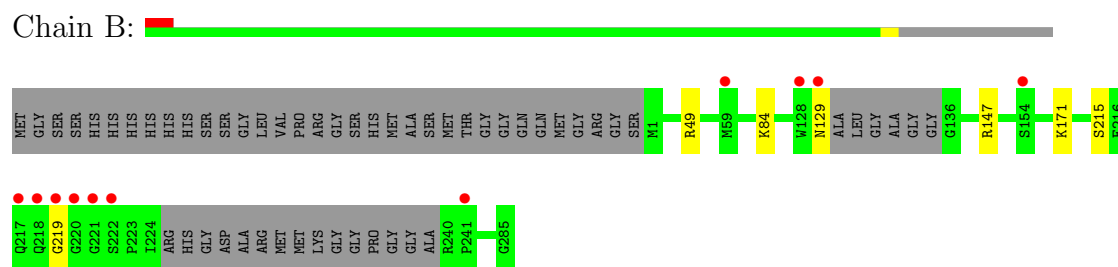
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



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) 97.3 (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 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
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 , 37.9	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38577 reflections	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.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2197	0	0	4	0
1	B	2050	0	0	5	0
2	C	85	0	0	1	0
2	D	85	0	0	2	0
3	A	27	0	0	0	0
3	B	27	0	0	0	0
4	A	8	0	6	0	0
5	A	1	0	0	0	0
6	A	190	0	0	2	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	6	11	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (11) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:84:LYS:NZ	6:B:2037:HOH:O	2.26	0.68
2:D:391:GHP:C6	2:D:393:3FG:N	2.75	0.50
1:B:129:ASN:ND2	6:B:2057:HOH:O	2.45	0.49
1:A:248:ARG:NH2	6:A:2160:HOH:O	2.46	0.48
1:B:147:ARG:NH1	6:B:2062:HOH:O	2.47	0.47
1:A:130:ALA:O	1:B:49:ARG:NH2	2.47	0.47
1:A:195:ASP:OD2	1:A:198:ARG:NH1	2.49	0.45
2:C:387:GHP:C2	2:C:389:3FG:CG2	2.96	0.43
2:D:391:GHP:C6	2:D:392:OMY:C	2.98	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	95	96
1	B	211/253 (83%)	210 (100%)	1 (0%)	94	94
All	All	436/506 (86%)	434 (100%)	2 (0%)	94	94

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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	GHP	C	387	2	11,11,12	6.25	8 (72%)	12,14,16	1.05	1 (8%)
2	3MY	C	388	2	13,13,14	4.66	5 (38%)	15,17,19	1.06	1 (6%)
2	3FG	C	389	2	12,12,13	6.00	8 (66%)	14,16,18	3.43	1 (7%)
2	GHP	C	390	2	11,11,12	6.64	8 (72%)	12,14,16	3.02	5 (41%)
2	GHP	C	391	2	11,11,12	6.35	7 (63%)	12,14,16	10.02	3 (25%)
2	OMY	C	392	2	14,14,15	5.05	4 (28%)	17,19,21	2.17	6 (35%)
2	3FG	C	393	2	13,13,13	3.94	5 (38%)	18,18,18	0.94	0
2	GHP	D	387	2	11,11,12	5.93	8 (72%)	12,14,16	1.05	1 (8%)
2	3MY	D	388	2	13,13,14	4.60	4 (30%)	15,17,19	2.12	3 (20%)
2	3FG	D	389	2	12,12,13	5.98	8 (66%)	14,16,18	9.74	1 (7%)
2	GHP	D	390	2	11,11,12	6.29	8 (72%)	12,14,16	9.93	4 (33%)
2	GHP	D	391	2	11,11,12	6.64	7 (63%)	12,14,16	10.94	4 (33%)
2	OMY	D	392	2	14,14,15	5.66	6 (42%)	17,19,21	2.79	6 (35%)
2	3FG	D	393	2	13,13,13	3.93	5 (38%)	18,18,18	1.19	2 (11%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3FG	D	393	2	-	0/8/8/8	0/1/1/1

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	392	OMY	O-C	18.80	1.24	1.11
2	D	391	GHP	O-C	18.08	1.23	1.11
2	C	387	GHP	O-C	17.00	1.23	1.11
2	C	390	GHP	O-C	16.97	1.23	1.11
2	C	392	OMY	O-C	16.54	1.22	1.11
2	C	391	GHP	O-C	16.53	1.22	1.11
2	D	387	GHP	O-C	16.12	1.22	1.11
2	D	389	3FG	O-C	16.02	1.22	1.11
2	D	390	GHP	O-C	15.89	1.22	1.11
2	C	388	3MY	O-C	15.84	1.22	1.11
2	D	388	3MY	O-C	15.74	1.22	1.11
2	C	389	3FG	O-C	15.67	1.22	1.11
2	D	393	3FG	CG1-CB	8.80	1.54	1.38
2	C	393	3FG	CG1-CB	8.77	1.54	1.38
2	C	389	3FG	CG2-CB	7.53	1.52	1.38
2	D	389	3FG	CG2-CB	7.28	1.51	1.38
2	D	393	3FG	CZ-CD1	6.99	1.50	1.39
2	D	391	GHP	C6-C1	6.95	1.51	1.39
2	D	392	OMY	CZ-CE1	6.95	1.46	1.39
2	C	393	3FG	CZ-CD1	6.89	1.50	1.39
2	C	391	GHP	C6-C1	6.87	1.50	1.39
2	C	390	GHP	C6-C1	6.69	1.50	1.39
2	C	392	OMY	CZ-CE1	6.63	1.46	1.39
2	D	390	GHP	C6-C1	6.61	1.50	1.39
2	D	393	3FG	CZ-CD2	6.53	1.49	1.39
2	C	393	3FG	CZ-CD2	6.39	1.49	1.39
2	D	390	GHP	C6-C5	6.01	1.50	1.38
2	C	390	GHP	C6-C5	5.96	1.50	1.38
2	C	389	3FG	CZ-CD1	5.67	1.48	1.39
2	D	391	GHP	C3-C2	5.64	1.49	1.38
2	C	389	3FG	CA-C	5.62	1.54	1.48
2	C	391	GHP	C3-C2	5.61	1.49	1.38
2	C	391	GHP	C5-C4	5.51	1.50	1.38
2	D	389	3FG	CZ-CD1	5.50	1.48	1.39
2	C	390	GHP	C3-C2	5.43	1.49	1.38
2	D	390	GHP	C2-C1	5.35	1.48	1.39
2	C	389	3FG	CG1-CD1	5.30	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	390	GHP	C3-C2	5.27	1.48	1.38
2	C	390	GHP	C3-C4	5.24	1.49	1.38
2	D	389	3FG	CA-C	5.23	1.54	1.48
2	D	389	3FG	CG1-CD1	5.18	1.47	1.39
2	C	387	GHP	C6-C1	4.98	1.47	1.39
2	C	390	GHP	C2-C1	4.97	1.47	1.39
2	D	391	GHP	C5-C4	4.93	1.49	1.38
2	D	391	GHP	C3-C4	4.92	1.49	1.38
2	C	391	GHP	C2-C1	4.91	1.47	1.39
2	C	387	GHP	C2-C1	4.89	1.47	1.39
2	C	389	3FG	CZ-CD2	4.83	1.47	1.39
2	D	387	GHP	C6-C1	4.77	1.47	1.39
2	C	393	3FG	CG2-CD2	4.74	1.46	1.39
2	C	387	GHP	C3-C2	4.70	1.47	1.38
2	D	391	GHP	C2-C1	4.69	1.47	1.39
2	D	387	GHP	C2-C1	4.58	1.46	1.39
2	C	391	GHP	C3-C4	4.56	1.48	1.38
2	D	393	3FG	CG2-CD2	4.56	1.46	1.39
2	D	389	3FG	CZ-CD2	4.44	1.46	1.39
2	C	390	GHP	C5-C4	4.43	1.48	1.38
2	D	387	GHP	CA-C	4.37	1.53	1.48
2	C	387	GHP	C6-C5	4.36	1.47	1.38
2	D	387	GHP	C3-C2	4.33	1.47	1.38
2	D	387	GHP	C6-C5	4.25	1.46	1.38
2	C	387	GHP	CA-C	4.22	1.53	1.48
2	D	390	GHP	C3-C4	4.21	1.47	1.38
2	C	387	GHP	C5-C4	4.11	1.47	1.38
2	D	390	GHP	C5-C4	4.08	1.47	1.38
2	C	392	OMY	CD2-CG	4.01	1.45	1.39
2	C	387	GHP	C3-C4	3.97	1.47	1.38
2	D	387	GHP	C5-C4	3.86	1.47	1.38
2	C	390	GHP	CA-C	3.68	1.52	1.48
2	D	392	OMY	CD2-CG	3.61	1.45	1.39
2	C	391	GHP	C6-C5	3.46	1.45	1.38
2	D	387	GHP	C3-C4	3.46	1.46	1.38
2	D	392	OMY	CD1-CG	3.37	1.44	1.38
2	D	390	GHP	CA-C	3.30	1.51	1.48
2	C	388	3MY	CZ-CE2	2.93	1.42	1.39
2	C	393	3FG	CG2-CB	2.76	1.43	1.38
2	D	393	3FG	CG2-CB	2.73	1.43	1.38
2	C	389	3FG	CG2-CD2	2.67	1.43	1.39
2	D	389	3FG	CG2-CD2	2.65	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	388	3MY	CZ-CE2	2.58	1.42	1.39
2	D	391	GHP	C6-C5	2.55	1.43	1.38
2	D	388	3MY	CD2-CG	2.50	1.43	1.39
2	C	392	OMY	CD1-CG	2.46	1.43	1.38
2	D	392	OMY	CA-C	2.43	1.52	1.48
2	D	388	3MY	CE1-CZ	2.36	1.44	1.39
2	C	389	3FG	CG1-CB	2.29	1.43	1.38
2	C	388	3MY	CA-C	2.25	1.52	1.48
2	C	388	3MY	CD2-CG	2.20	1.43	1.39
2	C	388	3MY	CE1-CZ	2.10	1.43	1.39
2	D	389	3FG	CG1-CB	2.10	1.42	1.38
2	D	392	OMY	CA-CB	-2.09	1.51	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	391	GHP	C-CA-N	-37.59	109.01	113.27
2	D	389	3FG	C-CA-N	-36.33	109.15	113.27
2	C	391	GHP	C-CA-N	-34.29	109.38	113.27
2	D	390	GHP	C-CA-N	-33.99	109.42	113.27
2	C	389	3FG	C-CA-N	12.50	114.68	113.27
2	C	390	GHP	C-CA-N	8.43	114.22	113.27
2	D	392	OMY	CD1-CE1-CZ	-7.46	117.25	121.13
2	C	392	OMY	CG-CB-CA	-6.16	102.62	111.75
2	D	388	3MY	CD2-CE2-CZ	-6.00	118.01	121.13
2	D	392	OMY	CE2-CZ-CE1	5.22	123.31	118.80
2	D	392	OMY	CG-CB-CA	-4.05	105.74	111.75
2	C	392	OMY	CE2-CZ-CE1	3.63	121.94	118.80
2	D	388	3MY	CE1-CZ-CE2	3.56	121.87	118.80
2	C	390	GHP	C6-C1-C2	3.43	122.89	118.33
2	D	390	GHP	C5-C6-C1	-3.39	117.61	121.20
2	D	393	3FG	C-CA-N	3.19	116.63	108.21
2	C	391	GHP	C5-C6-C1	-3.13	117.88	121.20
2	D	392	OMY	CD2-CG-CB	-3.09	116.35	120.75
2	C	392	OMY	CD1-CE1-CZ	-3.09	119.52	121.13
2	C	390	GHP	C5-C6-C1	-3.04	117.98	121.20
2	C	391	GHP	C6-C1-C2	2.95	122.25	118.33
2	D	388	3MY	C-CA-N	-2.91	110.92	113.83
2	D	392	OMY	CD2-CG-CD1	2.79	122.28	118.76
2	C	390	GHP	C3-C2-C1	-2.77	118.27	121.20
2	C	390	GHP	C2-C1-CA	-2.71	116.86	120.60
2	D	391	GHP	C3-C2-C1	-2.55	118.50	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	391	GHP	C6-C1-CA	-2.53	117.10	120.60
2	D	390	GHP	C6-C1-C2	2.51	121.66	118.33
2	D	391	GHP	C6-C1-C2	2.50	121.65	118.33
2	D	392	OMY	CE2-CD2-CG	-2.49	118.56	121.20
2	C	388	3MY	CD2-CE2-CZ	-2.16	120.00	121.13
2	C	392	OMY	CD2-CG-CD1	2.12	121.44	118.76
2	D	387	GHP	C3-C2-C1	-2.09	118.99	121.20
2	D	390	GHP	C3-C2-C1	-2.06	119.02	121.20
2	C	392	OMY	CD2-CE2-CZ	-2.06	118.25	120.50
2	D	393	3FG	OXT-C-CA	2.03	118.89	113.75
2	C	387	GHP	C6-C1-C2	2.01	121.00	118.33
2	C	392	OMY	ODE-CB-CA	2.00	114.13	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	PAP	A	286	-	29,29,33	1.22	3 (10%)	45,45,52	2.45	9 (20%)
4	ACT	A	287	-	1,3,3	1.18	0	0,3,3	0.00	-
4	ACT	A	288	-	1,3,3	1.21	0	0,3,3	0.00	-
3	PAP	B	286	-	29,29,33	1.23	3 (10%)	45,45,52	2.15	9 (20%)

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	-	-	0/15/31/37	0/1/3/3
4	ACT	A	287	-	-	0/0/0/0	0/0/0/0
4	ACT	A	288	-	-	0/0/0/0	0/0/0/0
3	PAP	B	286	-	-	0/15/31/37	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	286	PAP	PA-O3A	3.52	1.62	1.50
3	B	286	PAP	C5-C4	3.31	1.48	1.40
3	A	286	PAP	C4-N9	-3.30	1.32	1.37
3	A	286	PAP	PA-O3A	2.95	1.60	1.50
3	B	286	PAP	C4-N9	-2.64	1.33	1.37
3	A	286	PAP	C5-C4	2.53	1.46	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	286	PAP	O4'-C1'-N9	10.07	117.80	108.44
3	B	286	PAP	O4'-C1'-N9	8.17	116.04	108.44
3	A	286	PAP	N3-C2-N1	-7.17	122.72	128.71
3	B	286	PAP	N3-C2-N1	-5.35	124.23	128.71
3	A	286	PAP	N3-C4-N9	5.22	134.85	125.43
3	B	286	PAP	N3-C4-N9	5.11	134.66	125.43
3	A	286	PAP	C8-N9-C4	4.10	110.03	106.90
3	B	286	PAP	O3A-PA-O5'	-3.29	98.12	108.11
3	B	286	PAP	C4-C5-N7	-3.25	106.74	109.52
3	B	286	PAP	C5-C4-N3	-3.13	118.88	125.70
3	B	286	PAP	O2A-PA-O1A	2.75	120.78	110.82
3	A	286	PAP	C5-C4-N3	-2.58	120.08	125.70
3	A	286	PAP	C4-C5-N7	-2.47	107.41	109.52
3	A	286	PAP	C2-N1-C6	2.38	123.06	118.77
3	A	286	PAP	O4'-C1'-C2'	-2.22	103.36	106.77
3	B	286	PAP	C2-N3-C4	2.15	120.13	114.01
3	B	286	PAP	O4'-C1'-C2'	-2.12	103.52	106.77
3	A	286	PAP	C2'-C1'-N9	-2.02	108.08	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	-0.20	11 (3%) 38 38	14, 28, 69, 104	0
1	B	264/319 (82%)	-0.12	11 (4%) 35 33	19, 34, 80, 134	0
2	C	7/7 (100%)	-1.11	0 100 100	24, 28, 31, 35	0
2	D	7/7 (100%)	-0.71	0 100 100	23, 25, 31, 35	0
All	All	564/652 (86%)	-0.18	22 (3%) 37 37	14, 31, 72, 134	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	GLY	5.7
1	B	219	GLY	5.6
1	B	222	SER	4.9
1	B	59	MET	4.6
1	A	131	LEU	4.1
1	A	231	MET	3.6
1	B	221	GLY	3.2
1	B	154	SER	3.2
1	A	221	GLY	3.1
1	A	130	ALA	3.1
1	B	217	GLN	3.0
1	A	222	SER	2.9
1	A	220	GLY	2.9
1	B	128	TRP	2.7
1	B	129	ASN	2.7
1	A	152	SER	2.5
1	A	-31	SER	2.3
1	B	241	PRO	2.2
1	A	285	GLY	2.2
1	B	218	GLN	2.2
1	A	224	ILE	2.1
1	A	129	ASN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GHP	D	387	11/12	0.11	0.85	24,29,35,40	0
2	GHP	D	390	11/12	0.10	0.70	21,22,24,24	0
2	3FG	D	393	13/13	0.12	0.25	29,33,38,40	0
2	OMY	D	392	14/15	0.10	-0.05	22,25,29,68	1
2	3FG	D	389	12/13	0.09	-0.15	22,24,26,26	0
2	OMY	C	392	14/15	0.09	-0.28	22,24,26,66	0
2	GHP	C	387	11/12	0.09	-0.43	32,33,37,37	0
2	3FG	C	393	13/13	0.08	-0.49	27,30,34,36	0
2	GHP	D	391	11/12	0.07	-0.63	22,24,26,26	0
2	3FG	C	389	12/13	0.08	-0.73	24,29,35,38	0
2	GHP	C	391	11/12	0.08	-0.84	22,26,28,32	0
2	3MY	C	388	13/14	0.08	-0.89	25,27,32,60	0
2	3MY	D	388	13/14	0.09	-1.48	24,26,29,66	1
2	GHP	C	390	11/12	0.07	-1.88	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ACT	A	288	4/4	0.11	18.82	59,60,61,62	0
5	CL	A	289	1/1	0.10	10.61	65,65,65,65	0
4	ACT	A	287	4/4	0.17	9.69	69,70,70,72	0
3	PAP	A	286	27/31	0.16	0.67	16,20,22,23	0
3	PAP	B	286	27/31	0.08	-0.71	27,35,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.