



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:16 am GMT

PDB ID : 4AID
Title : Crystal structure of C. crescentus PNPase bound to RNase E recognition peptide
Authors : Hardwick, S.W.; Gubbey, T.; Hug, I.; Jenal, U.; Luisi, B.F.
Deposited on : 2012-02-09
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

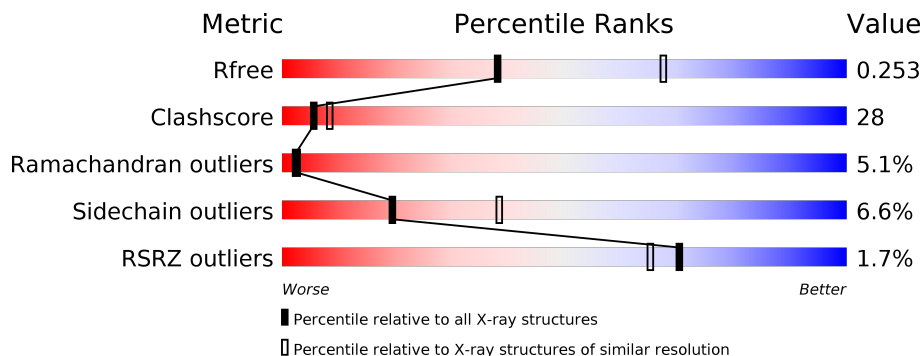
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	726	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>23%</div> <div>6%</div> <div>21%</div> </div> </div>
1	B	726	<div> <div>47%</div> <div>23%</div> <div>6%</div> <div>23%</div> </div>
1	C	726	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>26%</div> <div>26%</div> </div> </div>
2	F	14	<div> <div>14%</div> <div>21%</div> <div>7%</div> <div>7%</div> <div>50%</div> </div>
2	G	14	<div> <div>29%</div> <div>21%</div> <div>7%</div> <div>43%</div> </div>
2	H	14	<div> <div>29%</div> <div>7%</div> <div>64%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12655 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 POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	1	0
			4248	2686	720	819	23			
1	B	558	Total	C	N	O	S	0	0	0
			4170	2639	706	802	23			
1	C	539	Total	C	N	O	S	0	0	0
			3836	2425	654	735	22			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
A	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
A	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
A	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
A	0	PRO	-	EXPRESSION TAG	UNP Q9AC32
B	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
B	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
B	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
B	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
B	0	PRO	-	EXPRESSION TAG	UNP Q9AC32
C	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
C	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
C	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
C	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
C	0	PRO	-	EXPRESSION TAG	UNP Q9AC32

- Molecule 2 is a protein called RIBONUCLEASE, RNE/RNG FAMILY PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	0	0	0
			66	44	15	7			
2	G	8	Total	C	N	O	0	0	0
			77	50	19	8			
2	H	5	Total	C	N	O	0	0	0
			42	30	7	5			

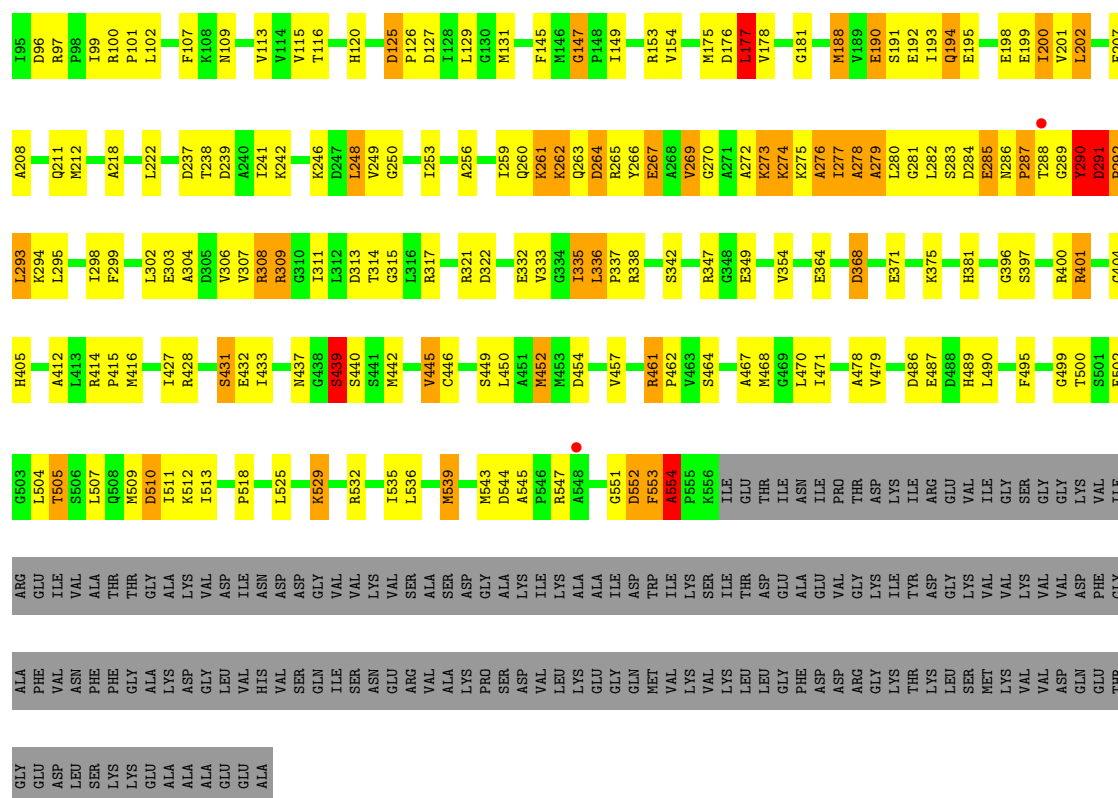
- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	80	Total	O	0	0
			80	80		
4	C	24	Total	O	0	0
			24	24		
4	G	1	Total	O	0	0
			1	1		



THR ASP LEU GLU ALA GLU VAL GLY LYS ILE TYR ASP GLY LYS VAL VAL VAL VAL ASP PHE GLY ALA PHE VAL ASN PHE PHE GLY ALA LYS ASP GLY LEU VAL HIS VAL SER GLN ILE SER ASN GLU ARG VAL ALA LYS PRO SER ASP VAL LEU LYS GLY GLN MET VAL VAL LYS

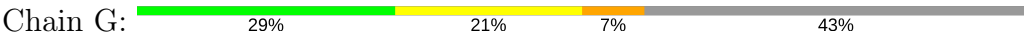
LEU LEU GLY PHE ASP ARG GLY LYS THR LYS LEU SER MET LYS VAL VAL ASP GLN GLU THR GLY GLU ASP LEU SER LYS LYS GLU ALA ALA GLU ALA

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR ALA PRO PRO GLU LYS R891 R892 R893 G894 W895 W896 R897 ARG

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR ALA PRO PRO GLU LYS R890 R891 R892 R893 G894 W895 W896 R897 ARG

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR ALA PRO PRO GLU LYS PRO ARG R893 W896 R897 ARG

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	157.44Å 157.44Å 302.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.60) 90.0 (29.75-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.254 0.209 , 0.253	Depositor DCC
R_{free} test set	2319 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 16.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.357 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12655	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	1.01	8/4324 (0.2%)	1.15	27/5859 (0.5%)
1	B	1.03	9/4242 (0.2%)	1.21	33/5744 (0.6%)
1	C	0.66	2/3900 (0.1%)	0.87	3/5305 (0.1%)
2	F	1.59	2/70 (2.9%)	1.32	1/94 (1.1%)
2	G	1.30	1/81 (1.2%)	1.14	0/109
2	H	1.49	1/45 (2.2%)	1.03	0/62
All	All	0.94	23/12662 (0.2%)	1.10	64/17173 (0.4%)

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
1	A	0	2
1	B	0	3
1	C	0	1
2	F	0	1
All	All	0	7

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	896	TRP	CD2-CE2	7.50	1.50	1.41
1	B	81	GLU	CD-OE1	6.69	1.33	1.25
2	G	896	TRP	CD2-CE2	6.34	1.49	1.41
1	A	432	GLU	CD-OE1	6.33	1.32	1.25
1	A	332	GLU	CD-OE1	6.26	1.32	1.25

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	LEU	CB-CG-CD1	-10.79	92.66	111.00
1	B	28	ASP	CB-CG-OD2	10.72	127.95	118.30
1	B	3	ASP	CB-CG-OD1	-10.37	108.97	118.30
1	B	153	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	B	486	ASP	CB-CG-OD1	-9.45	109.80	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	554	ALA	Peptide
1	A	8	THR	Peptide
1	B	554	ALA	Peptide
1	B	6	ARG	Peptide
1	B	9	ILE	Peptide

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	4248	0	4212	272	1
1	B	4170	0	4161	260	1
1	C	3836	0	3670	172	2
2	F	66	0	58	2	0
2	G	77	0	70	3	0
2	H	42	0	26	1	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
4	A	96	0	0	6	0
4	B	80	0	0	1	0
4	C	24	0	0	3	0
4	G	1	0	0	0	0
All	All	12655	0	12197	699	2

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 28.

The worst 5 of 699 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:287:PRO:HB2	1:A:288:THR:CG2	1.29	1.60
1:A:287:PRO:CB	1:A:288:THR:CG2	1.84	1.53
1:A:282:LEU:HA	1:A:292:PRO:CG	1.44	1.43
1:A:281:GLY:CA	1:A:289:GLY:O	1.68	1.37
1:B:274:LYS:HA	1:B:277:ILE:CG2	1.57	1.34

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:OG1	1:C:540:ASN:O[2_555]	1.87	0.33
1:B:6:ARG:NH2	1:C:224:GLU:OE2[3_565]	2.10	0.10

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	570/726 (78%)	502 (88%)	37 (6%)	31 (5%)	2	2
1	B	556/726 (77%)	490 (88%)	41 (7%)	25 (4%)	3	3
1	C	535/726 (74%)	476 (89%)	32 (6%)	27 (5%)	2	3
2	F	5/14 (36%)	4 (80%)	0	1 (20%)	0	0
2	G	6/14 (43%)	5 (83%)	0	1 (17%)	0	0
2	H	3/14 (21%)	2 (67%)	1 (33%)	0	100	100
All	All	1675/2220 (76%)	1479 (88%)	111 (7%)	85 (5%)	2	3

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ILE

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Mol	Chain	Res	Type
1	A	55	ASP
1	A	239	ASP
1	A	248	LEU
1	A	262	LYS

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	432/578 (75%)	401 (93%)	31 (7%)	17	33
1	B	428/578 (74%)	397 (93%)	31 (7%)	17	33
1	C	364/578 (63%)	348 (96%)	16 (4%)	33	60
2	F	5/12 (42%)	3 (60%)	2 (40%)	0	0
2	G	6/12 (50%)	5 (83%)	1 (17%)	2	4
2	H	2/12 (17%)	2 (100%)	0	100	100
All	All	1237/1770 (70%)	1156 (94%)	81 (6%)	19	39

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	64	GLN
1	B	242	LYS
1	C	496	LYS
1	B	83	ARG
1	B	188	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	GLN
1	B	119	GLN
1	C	225	HIS
1	B	109	ASN

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Mol	Chain	Res	Type
1	B	206	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](#)

3 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	$\# Z > 2$
3	PO4	A	1614	-	4,4,4	0.93	0	6,6,6	1.15	1 (16%)
3	PO4	B	1557	-	4,4,4	0.71	0	6,6,6	0.68	0
3	PO4	C	1556	-	4,4,4	0.72	0	6,6,6	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	1614	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1557	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	C	1556	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1614	PO4	O4-P-O3	2.01	115.30	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1614	PO4	1	0
3	B	1557	PO4	1	0
3	C	1556	PO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	573/726 (78%)	-0.42	11 (1%) 67 61	24, 34, 123, 161	0
1	B	558/726 (76%)	-0.47	2 (0%) 92 91	24, 33, 109, 147	0
1	C	539/726 (74%)	-0.11	15 (2%) 53 46	53, 87, 184, 253	0
2	F	7/14 (50%)	-0.23	0 100 100	40, 67, 84, 94	0
2	G	8/14 (57%)	-0.22	0 100 100	37, 68, 86, 93	0
2	H	5/14 (35%)	-0.07	0 100 100	82, 97, 103, 107	0
All	All	1690/2220 (76%)	-0.33	28 (1%) 70 65	24, 49, 135, 253	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	ALA	5.4
1	A	278	ALA	4.4
1	C	268	ALA	3.7
1	C	278	ALA	3.7
1	C	269	VAL	3.5

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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	C	1556	5/5	0.88	0.19	1.26	86,89,109,117	0
3	PO4	B	1557	5/5	0.97	0.10	-1.83	76,82,92,104	0
3	PO4	A	1614	5/5	0.98	0.10	-2.96	58,60,69,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.