



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:47 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

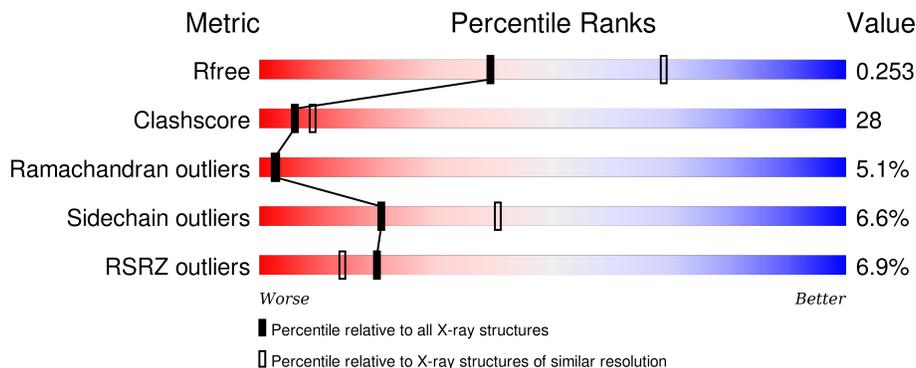
1 Overall quality at a glance i

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 48% 23% 6% • 21%</p>
1	B	726	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 47% 23% 6% • 23%</p>
1	C	726	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">11% 45% 26% • 26%</p>
2	F	14	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 14% 21% 7% 7% 50%</p>
2	G	14	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 29% 21% 7% 43%</p>

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Mol	Chain	Length	Quality of chain
2	H	14	 29% 7% 64%

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
3	PO4	C	1556	-	-	-	X

2 Entry composition i

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
			Total	C	N	O	S			
1	A	573	4248	2686	720	819	23	0	1	0
1	B	558	4170	2639	706	802	23	0	0	0
1	C	539	3836	2425	654	735	22	0	0	0

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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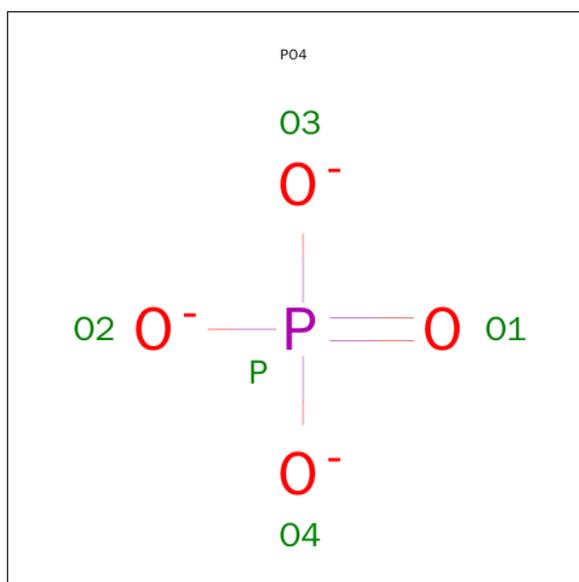
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
B	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
B	0	PRO	-	EXPRESSION 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 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

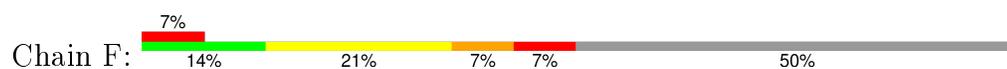
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	96	Total O 96 96	0	0
4	B	80	Total O 80 80	0	0
4	C	24	Total O 24 24	0	0
4	G	1	Total O 1 1	0	0

GLU
ILE
VAL
ALA
THR
THR
GLY
ALA
LYS
VAL
ASP
ILE
ASN
ASP
GLY
VAL
VAL
LYS
VAL
SER
ALA
SER
GLY
ALA
ILE
LYS
ALA
ALA
ILE
ASP
TRP
ILE
LYS
SER
ILE
THR
ASP
GLY
ALA
GLU
VAL
GLY
LYS
ILE
TYR
THR
ASP
GLY
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VAL
ASP
PHE
GLU
THR
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ALA

PHE
VAL
ASN
PHE
PHE
GLY
ALA
LYS
ASP
GLY
LEU
VAL
HIS
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GLN
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ASN
GLU
ARG
VAL
ALA
SER
LYS
PRO
SER
ASP
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LYS
LEU
LEU
PHE
ASP
ARG
ARG
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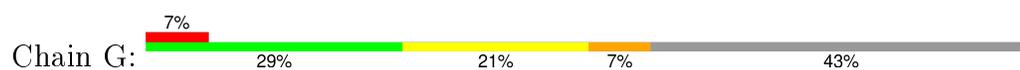
GLU
ASP
LEU
SER
LYS
GLU
ALA
ALA
GLU
ALA

- Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



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

- Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR
ALA
PRO
GLU
K890
R891
R892
R893
G894
W895
W896
R897
ARG

- Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR
ALA
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	2587 reflections (3.45%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.3	EDS
Estimated twinning fraction	0.357 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77316 reflections	Xtriage
F_o, F_c correlation	0.93	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 [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	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 4
1	C	535/726 (74%)	476 (89%)	32 (6%)	27 (5%)	3 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 [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	432/578 (75%)	401 (93%)	31 (7%)	18	35
1	B	428/578 (74%)	397 (93%)	31 (7%)	18	35
1	C	364/578 (63%)	348 (96%)	16 (4%)	35	63
2	F	5/12 (42%)	3 (60%)	2 (40%)	0	0
2	G	6/12 (50%)	5 (83%)	1 (17%)	3	4
2	H	2/12 (17%)	2 (100%)	0	100	100
All	All	1237/1770 (70%)	1156 (94%)	81 (6%)	21	42

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	0.25	0	6,6,6	0.33	0
3	PO4	B	1557	-	4,4,4	0.15	0	6,6,6	0.28	0
3	PO4	C	1556	-	4,4,4	0.31	0	6,6,6	0.29	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.

There are no bond angle outliers.

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%)	-0.09	25 (4%) 38 30	24, 34, 123, 161	0
1	B	558/726 (76%)	-0.23	12 (2%) 65 59	24, 33, 109, 147	0
1	C	539/726 (74%)	0.59	78 (14%) 3 2	53, 87, 184, 253	0
2	F	7/14 (50%)	0.56	1 (14%) 4 2	40, 67, 84, 94	0
2	G	8/14 (57%)	0.35	1 (12%) 5 3	37, 68, 86, 93	0
2	H	5/14 (35%)	0.33	0 100 100	82, 97, 103, 107	0
All	All	1690/2220 (76%)	0.09	117 (6%) 20 14	24, 49, 135, 253	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	6.3
1	C	270	GLY	6.2
1	C	269	VAL	5.7
1	C	297	ALA	5.5
1	C	271	ALA	5.4

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(Å ²)	Q<0.9
3	PO4	C	1556	5/5	0.81	0.29	5.60	86,89,109,117	0
3	PO4	B	1557	5/5	0.97	0.11	-1.34	76,82,92,104	0
3	PO4	A	1614	5/5	0.96	0.12	-1.54	58,60,69,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.