



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 4AID / pdb_00004aid
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

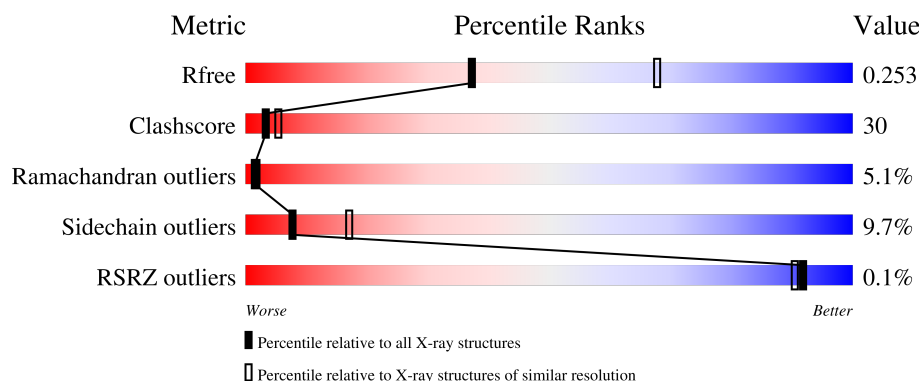
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of 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	726	
1	B	726	
1	C	726	
2	F	14	
2	G	14	

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Mol	Chain	Length	Quality of chain
2	H	14	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment on the left labeled '29%', a yellow segment in the middle labeled '7%', and a grey segment on the right labeled '64%'. The total length of the bar represents 100%.

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 (CCD ID: 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		

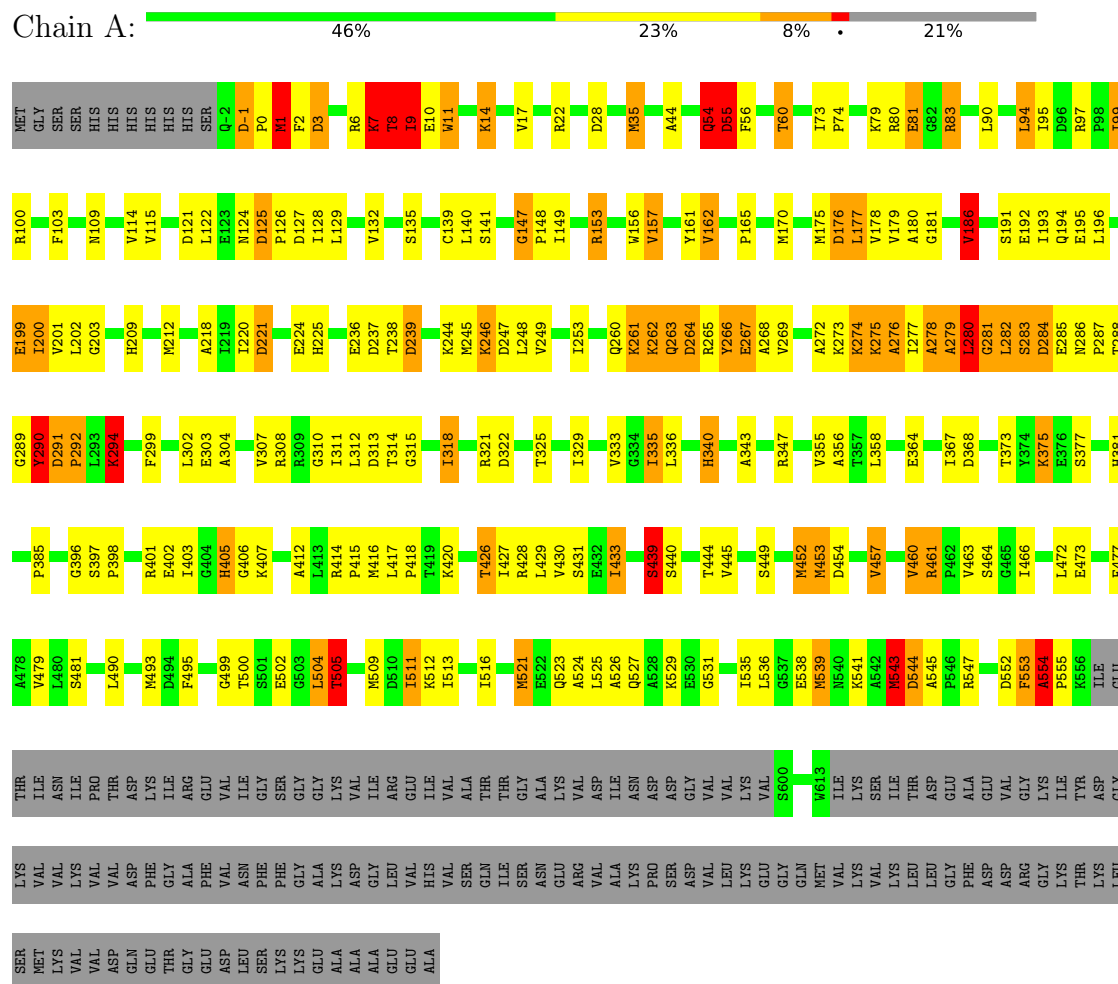
- Molecule 4 is water.

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		

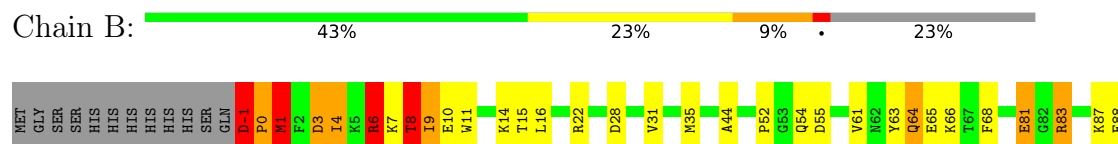
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE



• Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE



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

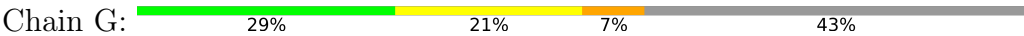
ARG
VAL
ALA
SER
PRO
GLY
SER
ASP
VAL
LEU
LYS
GLY
GLN
MET
VAL
LYS
VAL
LYS
LEU
LEU
GLY
PHE
ASP
ASP
ARG
GLY
LYS
THR
LYS
LEU
SER
MET
LYS
VAL
VAL
VAL
GLN
GLU
THR
GLY
GLU
ASP
LEU
SER
LYS
LYS
GLY
ALA
ALA
GLY
LEU
GLU
ALA

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR
ALA
PRO
PRO
GLY
LYS
P891
R892
R893
G894
W895
W896
R897
ARG

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR
ALA
PRO
PRO
GLY
P890
R891
R892
R893
G894
W895
W896
R897
ARG

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR
ALA
PRO
PRO
GLY
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 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.60) 90.0 (30.00-2.60)	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 (3.01%)	wwPDB-VP
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 , 18.8	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	0.95	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	1.35	21/4324 (0.5%)	1.49	46/5859 (0.8%)
1	B	1.39	18/4242 (0.4%)	1.51	65/5744 (1.1%)
1	C	0.94	2/3900 (0.1%)	1.21	20/5305 (0.4%)
2	F	1.49	1/70 (1.4%)	1.58	2/94 (2.1%)
2	G	1.18	0/81	1.42	1/109 (0.9%)
2	H	1.25	0/45	1.18	0/62
All	All	1.25	42/12662 (0.3%)	1.41	134/17173 (0.8%)

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 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	ASN	C-O	-11.03	1.18	1.23
1	A	7	LYS	CA-C	-9.33	1.43	1.52
1	B	7	LYS	CA-C	-8.39	1.42	1.52
1	B	338	ARG	N-CA	7.59	1.55	1.46
1	B	147	GLY	N-CA	7.25	1.54	1.44

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	LYS	N-CA-C	-12.51	96.71	112.72
1	B	7	LYS	N-CA-C	-11.69	95.97	114.09
1	A	9	ILE	N-CA-C	-11.46	85.50	109.34
1	A	553	PHE	N-CA-C	-10.36	93.29	109.76
1	C	-1	ASP	CA-C-N	-10.25	108.31	118.97

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	290	1
1	B	4170	0	4161	275	1
1	C	3836	0	3670	190	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	750	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 30.

The worst 5 of 750 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:A:493:MET:CE	1:A:509:MET:HE3	1.55	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

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	570/726 (78%)	502 (88%)	37 (6%)	31 (5%)	1	1
1	B	556/726 (77%)	490 (88%)	41 (7%)	25 (4%)	2	2
1	C	535/726 (74%)	476 (89%)	32 (6%)	27 (5%)	1	2
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%)	1	2

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%)	389 (90%)	43 (10%)	7	16
1	B	428/578 (74%)	382 (89%)	46 (11%)	6	14
1	C	364/578 (63%)	336 (92%)	28 (8%)	12	27
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%)	1117 (90%)	120 (10%)	8	17

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	188	MET
1	C	445	VAL
1	B	355	VAL
1	C	434	THR
2	F	897	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	206	ASN
1	B	405	HIS
1	C	523	GLN
1	B	381	HIS

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Mol	Chain	Res	Type
1	C	62	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 oligosaccharides 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	B	1557	-	4,4,4	0.73	0	6,6,6	0.81	0
3	PO4	A	1614	-	4,4,4	0.92	0	6,6,6	1.37	1 (16%)
3	PO4	C	1556	-	4,4,4	0.81	0	6,6,6	1.02	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1614	PO4	O4-P-O3	2.38	115.30	107.91
3	C	1556	PO4	O4-P-O2	2.26	114.96	107.91

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	B	1557	PO4	1	0
3	A	1614	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%)	-1.55	0	100 100	24, 34, 123, 161	1 (0%)
1	B	558/726 (76%)	-1.58	0	100 100	24, 33, 109, 147	0
1	C	539/726 (74%)	-0.78	1 (0%)	91 90	53, 87, 184, 253	0
2	F	7/14 (50%)	-1.07	0	100 100	40, 67, 84, 94	0
2	G	8/14 (57%)	-1.30	0	100 100	37, 68, 86, 93	0
2	H	5/14 (35%)	-0.75	0	100 100	82, 97, 103, 107	0
All	All	1690/2220 (76%)	-1.31	1 (0%)	92 90	24, 49, 135, 253	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	VAL	2.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
3	PO4	C	1556	5/5	0.98	0.10	86,89,109,117	0
3	PO4	B	1557	5/5	0.99	0.05	76,82,92,104	0
3	PO4	A	1614	5/5	0.99	0.04	58,60,69,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.