



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 01:56 PM EST

PDB ID : 3T7U  
Title : A NeW Crystal structure of APC-ARM  
Authors : Zhang, Z.; Wu, G.  
Deposited on : 2011-07-31  
Resolution : 2.90 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](mailto: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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

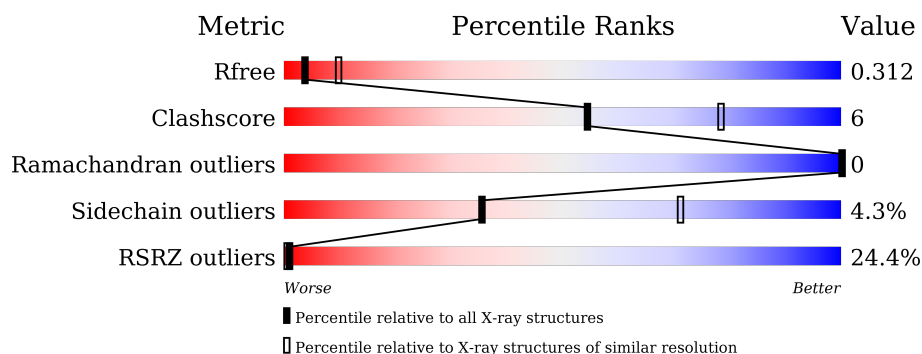
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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	378	<div> <div>20%</div> <div>67%</div> <div>14%</div> <div>•</div> <div>18%</div> </div>
1	B	378	<div> <div>20%</div> <div>70%</div> <div>11%</div> <div>•</div> <div>18%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4807 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 Adenomatous polyposis coli protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2381	1485	429	441	26			
1	B	311	Total	C	N	O	S	0	0	0
			2390	1491	431	442	26			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	MET	-	EXPRESSION TAG	UNP P25054
A	399	GLY	-	EXPRESSION TAG	UNP P25054
A	400	HIS	-	EXPRESSION TAG	UNP P25054
A	401	HIS	-	EXPRESSION TAG	UNP P25054
A	402	HIS	-	EXPRESSION TAG	UNP P25054
A	403	HIS	-	EXPRESSION TAG	UNP P25054
A	404	HIS	-	EXPRESSION TAG	UNP P25054
A	405	HIS	-	EXPRESSION TAG	UNP P25054
A	406	MET	-	EXPRESSION TAG	UNP P25054
B	398	MET	-	EXPRESSION TAG	UNP P25054
B	399	GLY	-	EXPRESSION TAG	UNP P25054
B	400	HIS	-	EXPRESSION TAG	UNP P25054
B	401	HIS	-	EXPRESSION TAG	UNP P25054
B	402	HIS	-	EXPRESSION TAG	UNP P25054
B	403	HIS	-	EXPRESSION TAG	UNP P25054
B	404	HIS	-	EXPRESSION TAG	UNP P25054
B	405	HIS	-	EXPRESSION TAG	UNP P25054
B	406	MET	-	EXPRESSION TAG	UNP P25054

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

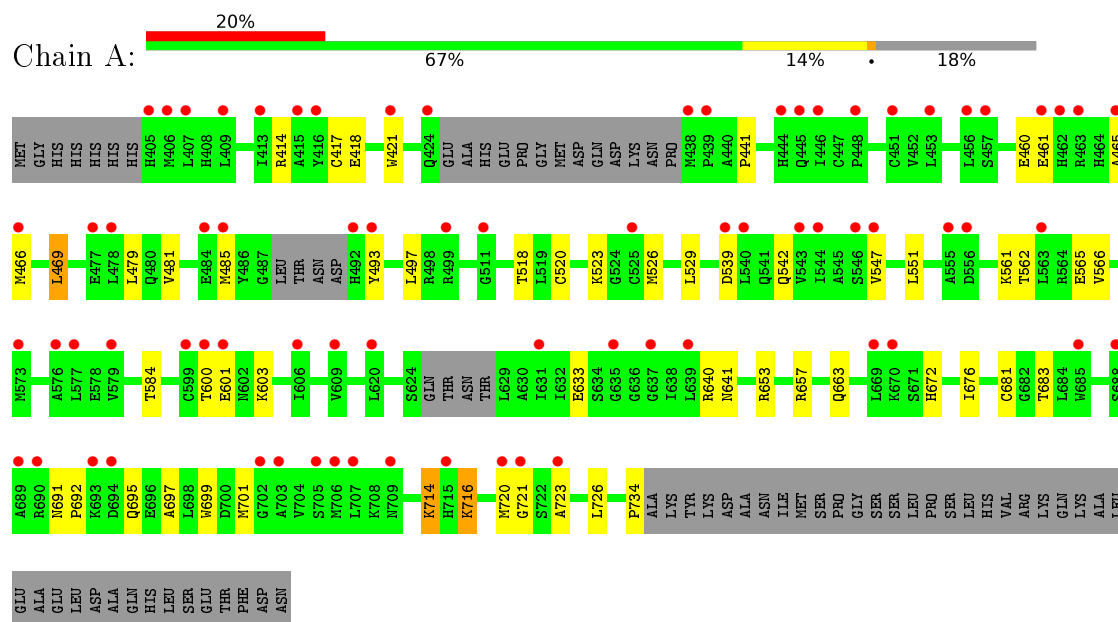
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	14	Total	O	0	0
			14	14		

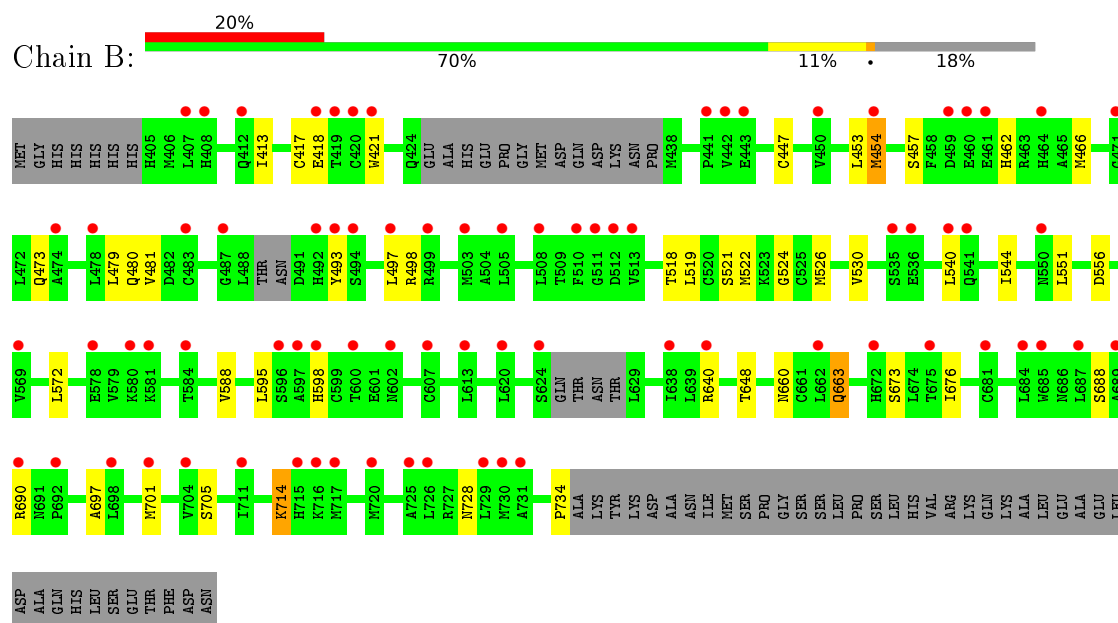
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Adenomatous polyposis coli protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.50 Å 72.50 Å 129.98 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 28.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	53.8 (30.00-2.90) 53.7 (28.86-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.87 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.269 , 0.313 0.269 , 0.312	Depositor DCC
$R_{free}$ test set	447 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 16.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.499 for h,-h-k,-l 0.107 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: 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	0.32	0/2413	0.50	1/3254 (0.0%)
1	B	0.33	0/2422	0.52	1/3267 (0.0%)
All	All	0.32	0/4835	0.51	2/6521 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	734	PRO	N-CA-CB	6.30	110.87	103.30
1	A	734	PRO	N-CA-CB	6.14	110.66	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2381	0	2407	34	0
1	B	2390	0	2408	38	0
2	A	10	0	0	1	0
3	A	12	0	0	0	0
3	B	14	0	0	0	0
All	All	4807	0	4815	61	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 6.

All (61) 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:697:ALA:O	1:B:701:MET:HG2	1.32	1.26
1:A:720:MET:HG3	1:B:421:TRP:HB3	1.19	1.18
1:B:454:MET:SD	1:B:454:MET:C	2.40	0.99
1:B:454:MET:SD	1:B:454:MET:O	2.30	0.89
1:A:720:MET:HG3	1:B:421:TRP:CB	2.06	0.80
1:A:720:MET:CG	1:B:421:TRP:HB3	2.08	0.80
1:B:518:THR:HG22	1:B:522:MET:CE	2.13	0.78
1:A:720:MET:HA	1:B:421:TRP:CE3	2.23	0.72
1:A:716:LYS:HZ2	1:B:421:TRP:HE1	1.38	0.71
1:B:518:THR:HG22	1:B:522:MET:HE3	1.72	0.70
1:A:603:LYS:HE3	1:A:641:ASN:O	1.92	0.69
1:A:681:CYS:HB3	1:A:721:GLY:HA3	1.74	0.68
1:B:697:ALA:O	1:B:701:MET:CG	2.27	0.67
1:B:413:ILE:HD11	1:B:453:LEU:HD13	1.75	0.66
1:A:723:ALA:HA	1:A:726:LEU:HB3	1.83	0.61
1:A:481:VAL:O	1:A:485:MET:HG2	2.01	0.60
1:A:523:LYS:HD3	1:A:562:THR:HG23	1.84	0.59
1:A:414:ARG:O	1:A:418:GLU:HG2	2.05	0.56
1:A:716:LYS:HZ1	1:B:481:VAL:HB	1.70	0.56
1:A:714:LYS:HG2	1:B:522:MET:HG2	1.86	0.56
1:B:413:ILE:HD11	1:B:453:LEU:CD1	2.36	0.56
1:A:542:GLN:HG2	1:A:584:THR:HA	1.87	0.56
1:B:648:THR:HG23	1:B:690:ARG:HH11	1.75	0.52
1:A:562:THR:O	1:A:566:VAL:HG22	2.10	0.52
1:A:465:ALA:O	1:A:469:LEU:HD12	2.10	0.51
1:B:518:THR:HG22	1:B:522:MET:HE2	1.91	0.51
1:A:520:CYS:O	1:A:562:THR:HG21	2.11	0.51
1:B:518:THR:O	1:B:522:MET:HG3	2.11	0.50
1:B:462:HIS:O	1:B:466:MET:HG2	2.12	0.50
1:A:716:LYS:O	1:A:720:MET:N	2.42	0.50
1:A:697:ALA:O	1:A:701:MET:HG3	2.11	0.49
1:A:600:THR:HA	1:A:603:LYS:HD2	1.94	0.48
1:B:595:LEU:O	1:B:598:HIS:HB2	2.15	0.47
1:A:653:ARG:O	1:A:657:ARG:HG3	2.15	0.47
1:A:723:ALA:HB3	1:B:418:GLU:OE2	2.16	0.46
1:B:454:MET:O	1:B:457:SER:OG	2.33	0.46
1:B:447:CYS:HB2	1:B:493:TYR:CE2	2.51	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:HB2	1:A:493:TYR:CD2	2.51	0.45
1:A:561:LYS:O	1:A:565:GLU:HG2	2.17	0.45
1:B:540:LEU:O	1:B:544:ILE:HG12	2.16	0.45
1:B:572:LEU:HD22	1:B:588:VAL:HG13	1.98	0.44
1:B:519:LEU:HD23	1:B:551:LEU:HD21	2.00	0.44
2:A:1:PO4:O4	1:B:524:GLY:N	2.51	0.43
1:A:633:GLU:HG3	1:A:676:ILE:HG13	2.00	0.43
1:A:526:MET:HA	1:A:529:LEU:HD12	2.00	0.43
1:A:714:LYS:HG3	1:B:522:MET:HE1	2.00	0.43
1:B:556:ASP:OD1	1:B:556:ASP:C	2.55	0.42
1:B:526:MET:O	1:B:530:VAL:HG23	2.19	0.42
1:B:688:SER:O	1:B:728:ASN:HB3	2.20	0.42
1:A:714:LYS:HB2	1:A:714:LYS:NZ	2.34	0.42
1:A:714:LYS:HD3	1:B:521:SER:OG	2.19	0.42
1:B:673:SER:HB3	1:B:676:ILE:HD12	2.01	0.42
1:B:660:ASN:HD21	1:B:663:GLN:HE21	1.68	0.41
1:A:716:LYS:HE2	1:B:480:GLN:HG2	2.01	0.41
1:B:714:LYS:CE	1:B:714:LYS:HA	2.51	0.41
1:A:547:VAL:O	1:A:551:LEU:HG	2.21	0.40
1:B:417:CYS:HB3	1:B:421:TRP:CZ2	2.56	0.40
1:A:695:GLN:O	1:A:699:TRP:HD1	2.04	0.40
1:A:417:CYS:HB3	1:A:421:TRP:CZ2	2.57	0.40
1:A:691:ASN:HA	1:A:692:PRO:HD3	1.92	0.40
1:B:479:LEU:HD23	1:B:498:ARG:HG2	2.03	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	301/378 (80%)	292 (97%)	9 (3%)	0	<b>100</b> <b>100</b>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	303/378 (80%)	292 (96%)	11 (4%)	0	100	100
All	All	604/756 (80%)	584 (97%)	20 (3%)	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	259/321 (81%)	244 (94%)	15 (6%)	25	58
1	B	258/321 (80%)	251 (97%)	7 (3%)	52	84
All	All	517/642 (80%)	495 (96%)	22 (4%)	35	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	GLU
1	A	461	GLU
1	A	466	MET
1	A	469	LEU
1	A	479	LEU
1	A	497	LEU
1	A	518	THR
1	A	539	ASP
1	A	601	GLU
1	A	640	ARG
1	A	663	GLN
1	A	672	HIS
1	A	683	THR
1	A	714	LYS
1	A	716	LYS
1	B	454	MET
1	B	473	GLN
1	B	497	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	640	ARG
1	B	663	GLN
1	B	705	SER
1	B	714	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	663	GLN
1	A	667	GLN
1	A	695	GLN
1	B	445	GLN
1	B	473	GLN
1	B	659	ASN
1	B	660	ASN
1	B	695	GLN

### 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](#)

2 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
2	PO4	A	1	-	4,4,4	0.75	0	6,6,6	0.23	0
2	PO4	A	2	-	4,4,4	0.74	0	6,6,6	0.23	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
2	PO4	A	1	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	309/378 (81%)	1.43	74 (23%) <b>1</b> <b>0</b>	35, 58, 84, 101	2 (0%)
1	B	311/378 (82%)	1.47	77 (24%) <b>1</b> <b>0</b>	35, 57, 84, 94	2 (0%)
All	All	620/756 (82%)	1.45	151 (24%) <b>1</b> <b>0</b>	35, 58, 84, 101	4 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	MET	9.0
1	A	493	TYR	6.9
1	B	672	HIS	6.3
1	B	464	HIS	5.4
1	B	421	TRP	5.4
1	B	513	VAL	5.3
1	A	693	LYS	4.9
1	A	445	GLN	4.9
1	B	461	GLU	4.6
1	A	405	HIS	4.5
1	B	442	VAL	4.4
1	A	609	VAL	4.3
1	A	707	LEU	4.3
1	B	536	GLU	4.2
1	B	493	TYR	4.0
1	B	443	GLU	4.0
1	A	448	PRO	4.0
1	B	535	SER	3.9
1	B	716	LYS	3.9
1	A	484	GLU	3.9
1	B	581	LYS	3.8
1	B	690	ARG	3.8
1	A	579	VAL	3.7
1	B	460	GLU	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	717	MET	3.7
1	A	721	GLY	3.7
1	B	584	THR	3.7
1	A	444	HIS	3.7
1	A	457	SER	3.7
1	A	706	MET	3.6
1	A	599	CYS	3.6
1	A	466	MET	3.5
1	B	726	LEU	3.5
1	A	453	LEU	3.4
1	A	556	ASP	3.4
1	A	639	LEU	3.3
1	B	541	GLN	3.3
1	B	607	CYS	3.3
1	A	635	GLY	3.3
1	A	463	ARG	3.3
1	A	461	GLU	3.3
1	A	540	LEU	3.3
1	B	510	PHE	3.2
1	B	471	GLY	3.2
1	A	409	LEU	3.2
1	B	613	LEU	3.2
1	A	669	LEU	3.2
1	B	459	ASP	3.1
1	B	503	MET	3.1
1	B	569	VAL	3.1
1	A	499	ARG	3.1
1	A	670	LYS	3.1
1	B	483	CYS	3.1
1	A	577	LEU	3.0
1	B	505	LEU	3.0
1	B	578	GLU	3.0
1	B	685	TRP	3.0
1	A	555	ALA	3.0
1	B	441	PRO	3.0
1	A	413	ILE	3.0
1	A	723	ALA	3.0
1	A	606	ILE	2.9
1	A	465	ALA	2.9
1	A	705	SER	2.8
1	B	600	THR	2.8
1	B	478	LEU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	685	TRP	2.8
1	A	547	VAL	2.8
1	A	406	MET	2.8
1	B	624	SER	2.8
1	A	525	CYS	2.8
1	B	602	ASN	2.8
1	B	408	HIS	2.8
1	B	420	CYS	2.8
1	A	539	ASP	2.7
1	B	698	LEU	2.7
1	A	702	GLY	2.7
1	A	492	HIS	2.7
1	B	730	MET	2.7
1	A	415	ALA	2.7
1	A	511	GLY	2.7
1	A	601	GLU	2.6
1	A	637	GLY	2.6
1	A	689	ALA	2.6
1	A	544	ILE	2.6
1	B	687	LEU	2.6
1	B	412	GLN	2.6
1	B	580	LYS	2.6
1	B	540	LEU	2.5
1	B	598	HIS	2.5
1	B	692	PRO	2.5
1	B	701	MET	2.5
1	B	704	VAL	2.5
1	B	512	ASP	2.5
1	B	494	SER	2.5
1	A	576	ALA	2.5
1	B	731	ALA	2.5
1	A	407	LEU	2.5
1	A	439	PRO	2.4
1	B	499	ARG	2.4
1	B	454	MET	2.4
1	B	419	THR	2.4
1	B	711	ILE	2.4
1	B	487	GLY	2.4
1	B	662	LEU	2.4
1	A	416	TYR	2.4
1	B	450	VAL	2.4
1	A	703	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	620	LEU	2.3
1	B	715	HIS	2.3
1	B	720	MET	2.3
1	B	620	LEU	2.3
1	A	477	GLU	2.3
1	B	418	GLU	2.3
1	B	407	LEU	2.3
1	B	689	ALA	2.3
1	A	446	ILE	2.3
1	A	631	ILE	2.3
1	B	596	SER	2.3
1	B	675	THR	2.3
1	A	715	HIS	2.2
1	B	550	ASN	2.2
1	B	497	LEU	2.2
1	B	511	GLY	2.2
1	A	478	LEU	2.2
1	B	508	LEU	2.2
1	B	640	ARG	2.2
1	A	451	CYS	2.2
1	B	681	CYS	2.2
1	A	563	LEU	2.2
1	B	729	LEU	2.2
1	A	424	GLN	2.2
1	A	456	LEU	2.2
1	B	725	ALA	2.2
1	A	546	SER	2.2
1	A	573	MET	2.2
1	A	421	TRP	2.2
1	A	688	SER	2.1
1	A	462	HIS	2.1
1	A	485	MET	2.1
1	A	720	MET	2.1
1	A	543	VAL	2.1
1	A	709	ASN	2.1
1	B	492	HIS	2.0
1	B	597	ALA	2.0
1	B	638	ILE	2.0
1	A	600	THR	2.0
1	A	690	ARG	2.0
1	A	694	ASP	2.0
1	B	684	LEU	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	474	ALA	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PO4	A	2	5/5	0.85	0.29	-0.93	64,65,65,65	0
2	PO4	A	1	5/5	0.93	0.16	-2.71	52,52,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.