



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:07 PM GMT

PDB ID : 4QLZ  
Title : The structure of inorganic pyrophosphatase from Schistosoma japonicum  
Authors : Wu, Q.F.  
Deposited on : 2014-06-13  
Resolution : 2.33 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.

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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-20026982  
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-20026982

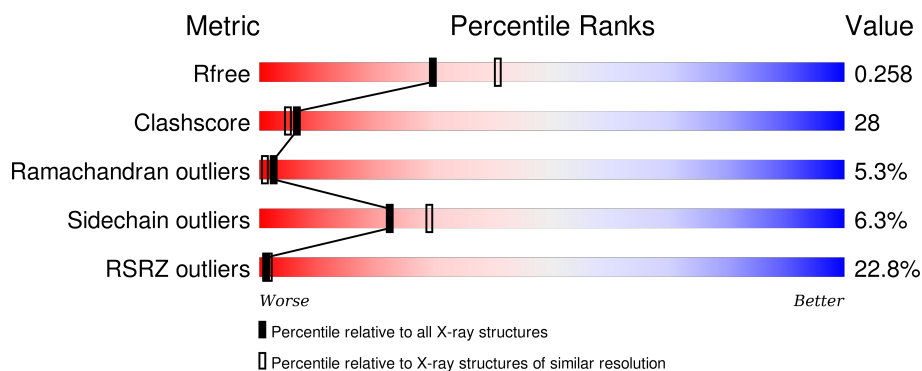
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	287	
1	B	287	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4628 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 SJCHGC07024 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2271	1458	377	424	12			
1	B	283	Total	C	N	O	S	0	0	0
			2259	1450	375	421	13			

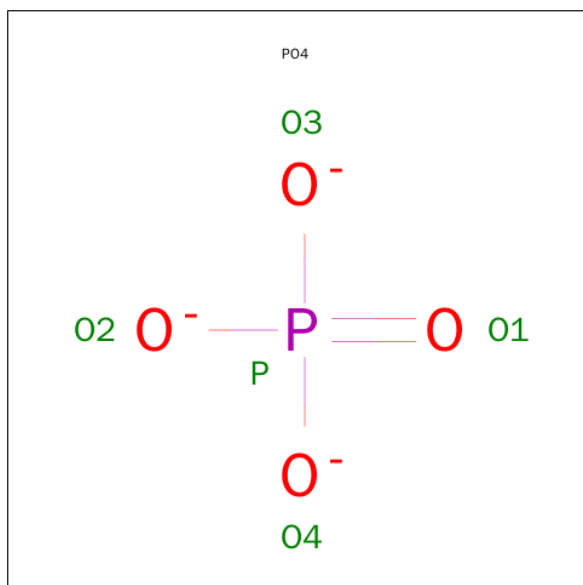
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ALA	VAL	ENGINEERED MUTATION	UNP Q5DE13
B	214	ALA	VAL	ENGINEERED MUTATION	UNP Q5DE13

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Co	0	0
			4	4		
2	A	4	Total	Co	0	0
			4	4		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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		

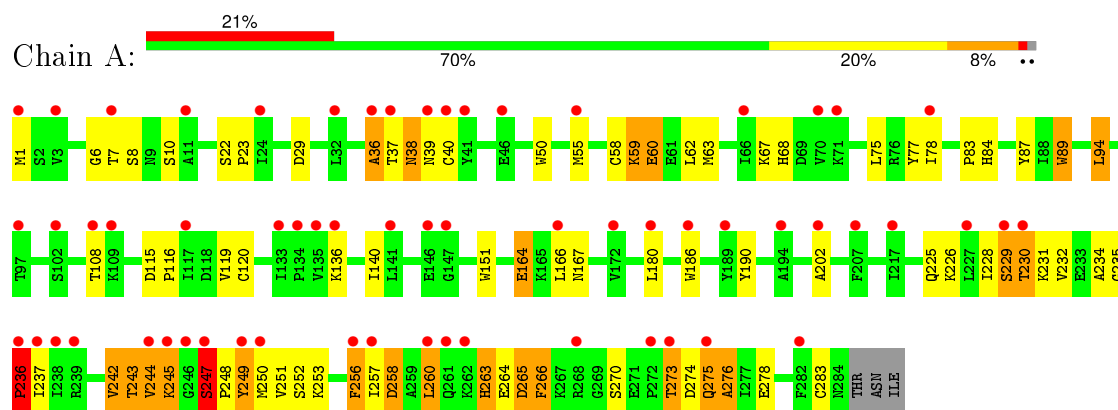
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	32	Total	O	0	0
			32	32		

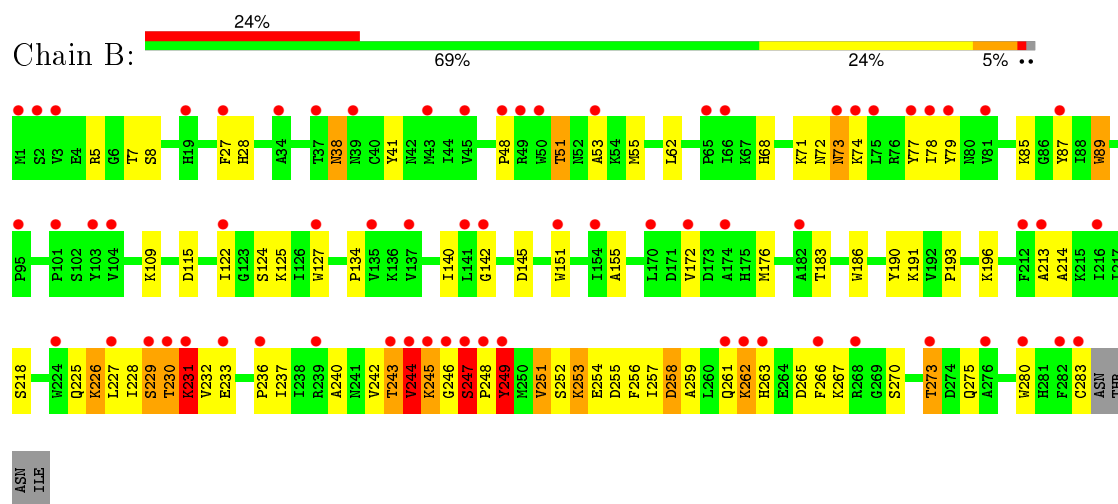
### 3 Residue-property plots [i](#)

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: SJCHGC07024 protein



#### • Molecule 1: SJCHGC07024 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.08 Å 76.08 Å 123.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.89 – 2.33 34.89 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.89-2.33) 98.4 (34.89-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.34 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.211 , 0.270 0.229 , 0.258	Depositor DCC
$R_{free}$ test set	1712 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.3	EDS
Estimated twinning fraction	0.012 for -h,-k,l 0.437 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 33781 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CO

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	0.49	0/2336	0.69	1/3168 (0.0%)
1	B	0.55	0/2323	0.68	2/3150 (0.1%)
All	All	0.52	0/4659	0.69	3/6318 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	247	SER	C-N-CD	-10.07	98.44	120.60
1	A	260	LEU	CB-CG-CD1	6.82	122.59	111.00
1	B	280	TRP	CA-CB-CG	5.46	124.06	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	GLU	Peptide
1	A	236	PRO	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	2271	0	2199	128	0
1	B	2259	0	2196	123	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	48	0	0	9	0
4	B	32	0	0	4	0
All	All	4628	0	4395	248	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 28.

All (248) 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:242:VAL:CG2	1:A:248:PRO:HG2	1.34	1.56
1:A:242:VAL:HG21	1:A:248:PRO:CG	1.35	1.53
1:A:242:VAL:CG2	1:A:248:PRO:CG	1.87	1.49
1:A:243:THR:HG23	1:A:244:VAL:CA	1.45	1.44
1:B:246:GLY:HA3	1:B:249:TYR:CD1	1.64	1.32
1:A:247:SER:HB3	1:A:248:PRO:CD	1.63	1.24
1:B:246:GLY:N	1:B:249:TYR:CZ	2.03	1.24
1:B:243:THR:HG23	1:B:244:VAL:N	1.57	1.13
1:B:246:GLY:HA2	1:B:249:TYR:CD2	1.83	1.13
1:A:244:VAL:HG22	1:A:245:LYS:HG3	1.25	1.12
1:B:246:GLY:HA3	1:B:249:TYR:CE1	1.86	1.10
1:A:243:THR:CG2	1:A:244:VAL:CA	2.30	1.10
1:A:243:THR:HG23	1:A:244:VAL:CB	1.82	1.10
1:A:243:THR:CG2	1:A:244:VAL:HA	1.82	1.08
1:B:244:VAL:HG13	1:B:245:LYS:H	1.10	1.08
1:A:242:VAL:CG2	1:A:248:PRO:CD	2.32	1.07
1:A:242:VAL:HG23	1:A:248:PRO:CD	1.82	1.07
1:A:243:THR:O	1:A:248:PRO:HD3	1.54	1.06
1:B:248:PRO:O	1:B:249:TYR:HB2	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG13	1:A:245:LYS:H	1.19	1.06
1:B:245:LYS:H	1:B:245:LYS:HE2	1.18	1.05
1:A:243:THR:HG23	1:A:244:VAL:HA	1.05	1.05
1:A:257:ILE:HG21	1:A:260:LEU:HD13	1.38	1.05
1:A:247:SER:CB	1:A:248:PRO:HD3	1.87	1.04
1:B:254:GLU:HG3	1:B:255:ASP:N	1.70	1.04
1:B:246:GLY:N	1:B:249:TYR:CE2	2.26	1.03
1:A:242:VAL:HG23	1:A:248:PRO:CG	1.82	1.02
1:A:244:VAL:N	1:A:247:SER:HB2	1.74	1.02
1:A:244:VAL:HG13	1:A:245:LYS:N	1.73	0.99
1:B:246:GLY:CA	1:B:249:TYR:CD2	2.45	0.99
1:B:245:LYS:HE2	1:B:245:LYS:N	1.77	0.98
1:B:246:GLY:HA3	1:B:249:TYR:CG	1.98	0.98
1:B:243:THR:HG23	1:B:244:VAL:H	1.15	0.98
1:B:244:VAL:HG13	1:B:245:LYS:N	1.78	0.98
1:B:245:LYS:C	1:B:249:TYR:CE2	2.38	0.97
1:A:244:VAL:H	1:A:247:SER:HB2	1.25	0.96
1:B:251:VAL:HG13	1:B:253:LYS:H	1.31	0.96
1:B:244:VAL:CG1	1:B:245:LYS:N	2.30	0.95
1:B:246:GLY:CA	1:B:249:TYR:CE2	2.49	0.95
1:A:243:THR:O	1:A:247:SER:HB3	1.67	0.95
1:B:246:GLY:CA	1:B:249:TYR:CG	2.50	0.95
1:B:28:HIS:HB2	1:B:242:VAL:HG12	1.51	0.93
1:A:242:VAL:CG2	1:A:248:PRO:HG3	1.98	0.93
1:B:246:GLY:CA	1:B:249:TYR:CD1	2.53	0.92
1:B:246:GLY:CA	1:B:249:TYR:CZ	2.54	0.90
1:A:247:SER:HB3	1:A:248:PRO:HD3	0.90	0.89
1:B:283:CYS:O	4:B:525:HOH:O	1.90	0.88
1:B:246:GLY:CA	1:B:249:TYR:CE1	2.57	0.88
1:A:244:VAL:CG1	1:A:245:LYS:H	1.82	0.88
1:A:251:VAL:HG22	1:A:253:LYS:H	1.40	0.87
1:A:242:VAL:HG23	1:A:243:THR:O	1.74	0.86
1:B:228:ILE:O	1:B:251:VAL:HG23	1.76	0.85
1:B:243:THR:CG2	1:B:244:VAL:N	2.29	0.85
1:A:140:ILE:HD11	1:A:151:TRP:HB3	1.58	0.83
1:A:244:VAL:CG2	1:A:245:LYS:HG3	2.09	0.82
1:A:243:THR:CG2	1:A:244:VAL:HB	2.08	0.81
1:A:23:PRO:HD2	1:A:260:LEU:HD12	1.61	0.81
1:A:243:THR:CG2	1:A:244:VAL:CB	2.58	0.81
1:B:251:VAL:HG13	1:B:253:LYS:N	1.95	0.80
1:B:245:LYS:O	1:B:245:LYS:CE	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLU:CG	1:B:255:ASP:N	2.43	0.80
1:A:243:THR:O	1:A:248:PRO:CD	2.29	0.80
1:A:242:VAL:CB	1:A:248:PRO:CG	2.60	0.79
1:A:243:THR:O	1:A:247:SER:CB	2.29	0.79
1:A:244:VAL:HG22	1:A:245:LYS:N	1.97	0.79
1:B:244:VAL:HG23	1:B:257:ILE:HD11	1.66	0.77
1:A:58:CYS:O	1:A:60:GLU:N	2.18	0.76
1:A:242:VAL:CB	1:A:248:PRO:HG2	2.11	0.76
1:B:245:LYS:O	1:B:245:LYS:HE3	1.84	0.76
1:A:242:VAL:HG21	1:A:248:PRO:CD	2.06	0.75
1:B:246:GLY:HA2	1:B:249:TYR:CG	2.17	0.75
1:B:28:HIS:CB	1:B:242:VAL:CG1	2.64	0.75
1:B:28:HIS:CB	1:B:242:VAL:HG12	2.17	0.75
1:B:228:ILE:HG13	1:B:251:VAL:HG21	1.67	0.74
1:A:244:VAL:HG22	1:A:245:LYS:CG	2.13	0.74
1:A:243:THR:CG2	1:A:244:VAL:N	2.51	0.72
1:A:230:THR:HA	1:A:252:SER:H	1.54	0.72
1:A:242:VAL:HG23	1:A:248:PRO:HD3	1.70	0.71
1:A:244:VAL:HG22	1:A:245:LYS:H	1.55	0.71
1:A:234:ALA:HA	1:A:236:PRO:HD2	1.72	0.71
1:A:8:SER:O	1:A:270:SER:OG	2.07	0.71
1:A:242:VAL:HG11	1:A:251:VAL:HG11	1.72	0.70
1:A:29:ASP:OD2	1:A:242:VAL:O	2.10	0.69
1:B:246:GLY:O	1:B:247:SER:HB2	1.93	0.69
1:A:276:ALA:HB3	4:A:527:HOH:O	1.91	0.69
1:A:228:ILE:O	1:A:230:THR:N	2.26	0.69
1:A:116:PRO:O	4:A:515:HOH:O	2.12	0.68
1:B:245:LYS:HE2	1:B:245:LYS:CA	2.23	0.68
1:A:242:VAL:HB	1:A:248:PRO:HG3	1.76	0.68
1:A:94:LEU:HD13	1:A:119:VAL:HG21	1.75	0.67
1:B:258:ASP:OD1	1:B:259:ALA:N	2.21	0.67
1:A:257:ILE:HG22	1:A:260:LEU:H	1.57	0.67
1:B:245:LYS:C	1:B:249:TYR:CZ	2.64	0.67
1:B:248:PRO:O	1:B:249:TYR:CB	2.30	0.66
1:A:244:VAL:CG2	1:A:245:LYS:H	2.07	0.66
1:B:242:VAL:CG2	1:B:248:PRO:HD2	2.25	0.66
1:B:246:GLY:N	1:B:249:TYR:CE1	2.63	0.66
1:A:243:THR:CB	1:A:244:VAL:HA	2.22	0.66
1:A:115:ASP:OD2	4:A:543:HOH:O	2.14	0.66
1:B:242:VAL:HG21	1:B:248:PRO:HD2	1.77	0.66
1:A:242:VAL:CB	1:A:248:PRO:HG3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HB	1:B:248:PRO:HD3	1.79	0.65
1:B:7:THR:HG22	1:B:270:SER:HB3	1.79	0.65
1:A:225:GLN:O	1:A:229:SER:HB3	1.98	0.64
1:B:228:ILE:O	1:B:251:VAL:CG2	2.45	0.64
1:A:276:ALA:O	4:A:527:HOH:O	2.15	0.64
1:A:229:SER:O	1:A:231:LYS:N	2.31	0.64
1:B:72:ASN:O	1:B:73:ASN:HB2	1.97	0.64
1:B:77:TYR:OH	4:B:531:HOH:O	2.13	0.64
1:A:242:VAL:CG2	1:A:248:PRO:HD2	2.24	0.64
1:A:248:PRO:O	1:A:251:VAL:HG12	1.97	0.64
1:A:257:ILE:CG2	1:A:260:LEU:H	2.11	0.64
1:B:28:HIS:HB3	1:B:242:VAL:HG11	1.79	0.63
1:B:213:ALA:O	1:B:214:ALA:HB3	1.97	0.62
1:B:28:HIS:HB3	1:B:242:VAL:CG1	2.30	0.62
1:B:259:ALA:N	4:B:517:HOH:O	2.32	0.62
1:B:231:LYS:O	1:B:231:LYS:HG3	2.00	0.62
1:B:73:ASN:C	1:B:74:LYS:HD3	2.19	0.61
1:B:245:LYS:HE2	1:B:245:LYS:O	2.00	0.61
1:B:258:ASP:HB2	1:B:261:GLN:OE1	2.00	0.61
1:A:247:SER:CB	1:A:248:PRO:CD	2.51	0.61
1:B:229:SER:OG	1:B:230:THR:N	2.34	0.60
1:B:244:VAL:HG13	1:B:245:LYS:HE2	1.83	0.60
1:B:245:LYS:CA	1:B:249:TYR:CE2	2.84	0.60
1:A:78:ILE:HG13	1:A:87:TYR:CE1	2.36	0.60
1:A:243:THR:C	1:A:247:SER:HB2	2.21	0.60
1:B:251:VAL:HG13	1:B:254:GLU:H	1.68	0.59
1:A:273:THR:HG22	1:A:274:ASP:H	1.68	0.58
1:A:242:VAL:O	1:A:243:THR:HB	2.03	0.57
1:A:275:GLN:NE2	4:A:530:HOH:O	1.97	0.57
1:A:228:ILE:O	1:A:251:VAL:HG23	2.04	0.57
1:A:244:VAL:H	1:A:247:SER:CB	2.10	0.56
1:B:244:VAL:HG22	1:B:245:LYS:NZ	2.19	0.56
1:A:242:VAL:HG22	1:A:243:THR:N	2.20	0.56
1:B:28:HIS:HB2	1:B:242:VAL:CG1	2.26	0.56
1:A:242:VAL:CG2	1:A:243:THR:N	2.69	0.56
1:A:36:ALA:HB3	1:A:38:ASN:OD1	2.04	0.56
1:B:62:LEU:HD23	1:B:261:GLN:HG3	1.88	0.55
1:B:254:GLU:HG3	1:B:255:ASP:H	1.65	0.55
1:B:240:ALA:HB3	1:B:253:LYS:HG2	1.89	0.55
1:B:246:GLY:HA2	1:B:249:TYR:CE2	2.22	0.54
1:A:275:GLN:N	4:A:518:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:CG1	1:B:254:GLU:N	2.71	0.54
1:B:71:LYS:HD2	1:B:72:ASN:H	1.73	0.54
1:B:5:ARG:NE	1:B:262:LYS:HZ1	2.06	0.54
1:B:55:MET:HE3	1:B:68:HIS:CE1	2.43	0.53
1:A:251:VAL:HG22	1:A:253:LYS:N	2.18	0.53
1:A:228:ILE:HG12	1:A:251:VAL:HG21	1.90	0.53
1:B:225:GLN:O	1:B:229:SER:N	2.29	0.53
1:B:245:LYS:C	1:B:245:LYS:HE2	2.30	0.52
1:B:251:VAL:HG13	1:B:254:GLU:N	2.25	0.52
1:B:226:LYS:O	1:B:231:LYS:HG2	2.10	0.52
1:A:244:VAL:N	1:A:247:SER:CB	2.61	0.52
1:A:243:THR:C	1:A:247:SER:CB	2.78	0.52
1:B:243:THR:O	1:B:247:SER:O	2.27	0.51
1:A:257:ILE:HG21	1:A:260:LEU:CD1	2.26	0.51
1:A:229:SER:C	1:A:231:LYS:N	2.64	0.51
1:B:8:SER:O	1:B:270:SER:OG	2.13	0.51
1:B:48:PRO:O	1:B:51:THR:HB	2.11	0.51
1:A:108:THR:HG22	1:A:202:ALA:HB2	1.93	0.50
1:A:77:TYR:CZ	1:A:273:THR:HG21	2.47	0.50
1:A:235:GLY:N	1:A:236:PRO:HD2	2.26	0.50
1:B:78:ILE:HG12	1:B:87:TYR:CE1	2.47	0.50
1:B:244:VAL:HG22	1:B:245:LYS:HZ3	1.77	0.50
1:A:68:HIS:ND1	1:A:75:LEU:HD13	2.27	0.50
1:A:244:VAL:CG1	1:A:245:LYS:N	2.43	0.49
1:B:261:GLN:C	1:B:263:HIS:H	2.16	0.49
1:A:77:TYR:CE2	1:A:273:THR:HG21	2.47	0.49
1:B:71:LYS:HD2	1:B:72:ASN:N	2.28	0.49
1:A:78:ILE:HG13	1:A:87:TYR:HE1	1.75	0.49
1:A:243:THR:HG22	1:A:244:VAL:N	2.24	0.49
1:B:243:THR:O	1:B:244:VAL:O	2.30	0.48
1:A:136:LYS:NZ	1:A:164:GLU:HB3	2.28	0.48
1:B:140:ILE:HD11	1:B:151:TRP:HB3	1.95	0.48
1:B:172:VAL:HG13	1:B:176:MET:HE3	1.95	0.48
1:B:55:MET:HE1	1:B:68:HIS:HA	1.95	0.48
1:A:58:CYS:O	1:A:58:CYS:SG	2.71	0.48
1:B:243:THR:O	1:B:247:SER:HB3	2.14	0.47
1:A:38:ASN:O	1:A:40:CYS:N	2.47	0.47
1:B:242:VAL:HB	1:B:248:PRO:CD	2.44	0.47
1:A:258:ASP:N	1:A:258:ASP:OD1	2.45	0.47
1:A:264:GLU:O	1:A:266:PHE:N	2.43	0.47
1:A:242:VAL:HG21	1:A:248:PRO:HG2	0.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PHE:HA	1:B:257:ILE:HA	1.60	0.47
1:B:225:GLN:O	1:B:229:SER:HB3	2.15	0.47
1:A:274:ASP:N	1:A:274:ASP:OD1	2.48	0.47
1:A:1:MET:N	4:A:526:HOH:O	2.47	0.47
1:A:232:VAL:O	1:A:232:VAL:HG23	2.15	0.47
1:A:244:VAL:CG2	1:A:245:LYS:N	2.60	0.47
1:B:245:LYS:HB2	1:B:249:TYR:HE2	1.79	0.47
1:B:41:TYR:O	1:B:134:PRO:HA	2.14	0.46
1:A:23:PRO:HD2	1:A:260:LEU:CD1	2.38	0.46
1:A:256:PHE:C	1:A:257:ILE:HD12	2.35	0.46
1:A:276:ALA:N	4:A:518:HOH:O	2.49	0.46
1:A:50:TRP:CZ3	1:B:85:LYS:HD3	2.51	0.46
1:B:89:TRP:HD1	1:B:122:ILE:HG22	1.80	0.46
1:B:251:VAL:CG1	1:B:254:GLU:H	2.27	0.45
1:B:38:ASN:OD1	1:B:38:ASN:O	2.34	0.45
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.84	0.45
1:A:136:LYS:HZ3	1:A:164:GLU:HB3	1.81	0.45
1:B:246:GLY:O	1:B:247:SER:CB	2.64	0.45
1:B:231:LYS:O	1:B:233:GLU:N	2.50	0.45
1:B:191:LYS:HB3	1:B:196:LYS:HB2	1.99	0.45
1:B:246:GLY:N	1:B:249:TYR:OH	2.47	0.45
1:A:249:TYR:HB3	1:A:250:MET:H	1.52	0.44
1:B:186:TRP:O	1:B:190:TYR:HB3	2.17	0.44
1:A:59:LYS:HG3	1:A:60:GLU:OE2	2.17	0.44
1:B:53:ALA:HB1	1:B:55:MET:HE3	1.99	0.44
1:A:6:GLY:HA2	1:A:265:ASP:CG	2.38	0.44
1:B:89:TRP:CZ2	1:B:183:THR:HG23	2.53	0.44
1:B:55:MET:HE3	1:B:68:HIS:ND1	2.32	0.44
1:B:109:LYS:HA	1:B:109:LYS:HD3	1.74	0.44
1:A:186:TRP:O	1:A:190:TYR:HB3	2.18	0.43
1:A:242:VAL:O	1:A:243:THR:CB	2.63	0.43
1:A:22:SER:HA	1:A:23:PRO:HD2	1.82	0.43
1:B:74:LYS:N	1:B:74:LYS:HD3	2.34	0.43
1:A:55:MET:HE3	1:A:68:HIS:CE1	2.53	0.43
1:B:245:LYS:HA	1:B:246:GLY:HA2	1.73	0.43
1:B:79:TYR:CD2	1:B:193:PRO:HG2	2.53	0.43
1:A:37:THR:O	1:A:37:THR:HG22	2.18	0.43
1:A:242:VAL:HG23	1:A:248:PRO:HG3	1.76	0.42
1:A:50:TRP:CE3	1:B:85:LYS:HD3	2.53	0.42
1:A:83:PRO:HD2	1:A:84:HIS:CE1	2.54	0.42
1:A:58:CYS:SG	1:A:67:LYS:HD2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:C	1:A:231:LYS:H	2.22	0.42
1:A:276:ALA:C	4:A:527:HOH:O	2.55	0.42
1:A:263:HIS:CD2	1:A:266:PHE:HE1	2.37	0.42
1:B:267:LYS:HB3	1:B:267:LYS:HE3	1.81	0.42
1:B:258:ASP:CG	4:B:517:HOH:O	2.57	0.42
1:A:7:THR:HG22	1:A:270:SER:HB3	2.01	0.42
1:A:164:GLU:HA	1:A:166:LEU:H	1.84	0.42
1:B:261:GLN:N	1:B:261:GLN:OE1	2.45	0.42
1:B:142:GLY:HA2	1:B:151:TRP:CE3	2.54	0.42
1:B:262:LYS:HD2	1:B:262:LYS:HA	1.81	0.42
1:B:227:LEU:HA	1:B:231:LYS:HD2	2.02	0.41
1:A:62:LEU:HD12	1:A:63:MET:H	1.85	0.41
1:A:23:PRO:CD	1:A:260:LEU:HD12	2.41	0.41
1:B:244:VAL:HG12	1:B:245:LYS:N	2.25	0.41
1:A:242:VAL:HB	1:A:248:PRO:CG	2.38	0.41
1:B:125:LYS:HG2	1:B:127:TRP:CE2	2.56	0.41
1:A:278:GLU:HB3	1:B:124:SER:O	2.21	0.41
1:A:89:TRP:CG	1:A:120:CYS:HB3	2.55	0.41
1:A:62:LEU:HD12	1:A:63:MET:N	2.36	0.41
1:B:266:PHE:N	1:B:266:PHE:HD1	2.19	0.41
1:B:214:ALA:O	1:B:218:SER:HB3	2.21	0.40
1:B:122:ILE:HG12	1:B:155:ALA:O	2.21	0.40
1:B:244:VAL:C	1:B:245:LYS:HG3	2.42	0.40
1:B:266:PHE:N	1:B:266:PHE:CD1	2.89	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	282/287 (98%)	252 (89%)	15 (5%)	15 (5%)	<b>2</b> <b>1</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	281/287 (98%)	249 (89%)	17 (6%)	15 (5%)	2	1
All	All	563/574 (98%)	501 (89%)	32 (6%)	30 (5%)	2	1

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ALA
1	A	39	ASN
1	A	59	LYS
1	A	229	SER
1	A	230	THR
1	A	236	PRO
1	A	247	SER
1	A	256	PHE
1	A	265	ASP
1	A	275	GLN
1	B	73	ASN
1	B	145	ASP
1	B	237	ILE
1	B	244	VAL
1	B	247	SER
1	A	249	TYR
1	B	231	LYS
1	B	275	GLN
1	A	276	ALA
1	B	258	ASP
1	A	266	PHE
1	B	229	SER
1	B	249	TYR
1	B	265	ASP
1	A	244	VAL
1	B	262	LYS
1	B	273	THR
1	B	236	PRO
1	B	232	VAL
1	A	237	ILE

### 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	245/251 (98%)	230 (94%)	15 (6%)	23	30
1	B	244/251 (97%)	228 (93%)	16 (7%)	21	26
All	All	489/502 (97%)	458 (94%)	31 (6%)	22	29

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	38	ASN
1	A	60	GLU
1	A	89	TRP
1	A	94	LEU
1	A	167	ASN
1	A	226	LYS
1	A	242	VAL
1	A	243	THR
1	A	245	LYS
1	A	247	SER
1	A	258	ASP
1	A	263	HIS
1	A	273	THR
1	A	283	CYS
1	B	27	PHE
1	B	38	ASN
1	B	51	THR
1	B	89	TRP
1	B	115	ASP
1	B	226	LYS
1	B	230	THR
1	B	231	LYS
1	B	243	THR
1	B	244	VAL
1	B	245	LYS
1	B	249	TYR
1	B	251	VAL
1	B	252	SER
1	B	253	LYS
1	B	273	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	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](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	PO4	A	405	2	4,4,4	0.79	0	6,6,6	0.24	0
3	PO4	B	405	2	4,4,4	0.78	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
3	PO4	A	405	2	-	0/0/0/0	0/0/0/0
3	PO4	B	405	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.

No monomer is involved in short contacts.

## 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	284/287 (98%)	1.38	61 (21%)  	24, 63, 104, 145	0
1	B	283/287 (98%)	1.41	68 (24%)  	24, 62, 104, 127	0
All	All	567/574 (98%)	1.39	129 (22%)  	24, 62, 104, 145	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	23.0
1	B	244	VAL	11.3
1	A	37	THR	10.7
1	B	246	GLY	9.6
1	B	266	PHE	9.0
1	A	244	VAL	7.1
1	A	246	GLY	6.9
1	A	256	PHE	6.2
1	B	245	LYS	6.2
1	A	24	ILE	6.2
1	B	261	GLN	5.6
1	A	194	ALA	5.4
1	A	245	LYS	5.1
1	A	236	PRO	4.9
1	B	212	PHE	4.5
1	B	230	THR	4.4
1	A	261	GLN	4.2
1	B	75	LEU	4.2
1	A	268	ARG	4.1
1	B	151	TRP	4.0
1	A	78	ILE	4.0
1	A	70	VAL	4.0
1	B	74	LYS	3.9
1	B	79	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	137	VAL	3.9
1	A	260	LEU	3.8
1	A	3	VAL	3.8
1	A	46	GLU	3.8
1	A	250	MET	3.7
1	B	103	TYR	3.7
1	B	273	THR	3.7
1	B	87	TYR	3.6
1	B	73	ASN	3.6
1	B	66	ILE	3.5
1	B	231	LYS	3.5
1	B	53	ALA	3.5
1	B	247	SER	3.5
1	A	229	SER	3.4
1	B	268	ARG	3.4
1	B	280	TRP	3.3
1	B	142	GLY	3.3
1	A	147	GLY	3.3
1	B	249	TYR	3.2
1	B	104	VAL	3.2
1	B	248	PRO	3.2
1	B	50	TRP	3.1
1	A	102	SER	3.1
1	B	236	PRO	3.1
1	B	172	VAL	3.1
1	A	97	THR	3.1
1	A	108	THR	3.1
1	B	81	VAL	3.1
1	A	247	SER	3.1
1	A	189	TYR	3.0
1	B	127	TRP	3.0
1	A	133	ILE	3.0
1	B	262	LYS	3.0
1	B	141	LEU	3.0
1	B	170	LEU	3.0
1	B	229	SER	2.9
1	B	1	MET	2.9
1	B	233	GLU	2.8
1	A	66	ILE	2.8
1	A	135	VAL	2.8
1	B	3	VAL	2.8
1	A	249	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	45	VAL	2.7
1	B	65	PRO	2.7
1	A	186	TRP	2.7
1	B	34	ALA	2.7
1	B	174	ALA	2.7
1	A	109	LYS	2.7
1	B	182	ALA	2.7
1	B	239	ARG	2.7
1	A	11	ALA	2.6
1	A	238	ILE	2.6
1	A	136	LYS	2.6
1	A	272	PRO	2.5
1	A	71	LYS	2.5
1	A	32	LEU	2.5
1	A	41	TYR	2.5
1	A	141	LEU	2.5
1	B	19	HIS	2.4
1	A	237	ILE	2.4
1	A	40	CYS	2.4
1	B	39	ASN	2.4
1	B	216	ILE	2.4
1	B	2	SER	2.4
1	A	275	GLN	2.4
1	B	154	ILE	2.4
1	A	134	PRO	2.4
1	A	202	ALA	2.4
1	B	135	VAL	2.4
1	B	227	LEU	2.3
1	A	55	MET	2.3
1	B	282	PHE	2.3
1	B	78	ILE	2.3
1	A	180	LEU	2.3
1	A	39	ASN	2.3
1	A	273	THR	2.3
1	A	217	ILE	2.3
1	A	117	ILE	2.2
1	B	283	CYS	2.2
1	A	207	PHE	2.2
1	B	48	PRO	2.2
1	B	49	ARG	2.2
1	B	77	TYR	2.2
1	A	282	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	276	ALA	2.2
1	A	1	MET	2.2
1	A	172	VAL	2.2
1	A	257	ILE	2.2
1	B	27	PHE	2.1
1	B	224	TRP	2.1
1	A	36	ALA	2.1
1	B	213	ALA	2.1
1	A	166	LEU	2.1
1	B	95	PRO	2.1
1	A	146	GLU	2.1
1	A	7	THR	2.1
1	B	263	HIS	2.1
1	A	239	ARG	2.0
1	A	227	LEU	2.0
1	B	43	MET	2.0
1	B	243	THR	2.0
1	B	101	PRO	2.0
1	A	262	LYS	2.0
1	B	122	ILE	2.0
1	B	37	THR	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	CO	A	404	1/1	0.82	0.18	0.13	77,77,77,77	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO	A	402	1/1	0.86	0.16	-0.48	69,69,69,69	1
3	PO4	B	405	5/5	0.91	0.18	-0.65	38,40,52,57	5
3	PO4	A	405	5/5	0.97	0.14	-0.80	38,43,56,82	5
2	CO	B	401	1/1	0.87	0.16	-1.26	79,79,79,79	1
2	CO	B	402	1/1	0.95	0.15	-1.37	67,67,67,67	1
2	CO	B	404	1/1	0.75	0.12	-2.30	79,79,79,79	1
2	CO	A	401	1/1	0.86	0.13	-3.07	114,114,114,114	0
2	CO	A	403	1/1	0.85	0.19	-	110,110,110,110	1
2	CO	B	403	1/1	0.56	0.26	-	112,112,112,112	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.