



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:47 PM GMT

PDB ID : 4MQ2  
Title : The crystal structure of DYRK1a with a bound pyrido[2,3-d]pyrimidine inhibitor  
Authors : Lukacs, C.M.; Janson, C.A.; Garvie, C.; Liang, L.  
Deposited on : 2013-09-15  
Resolution : 2.80 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 (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

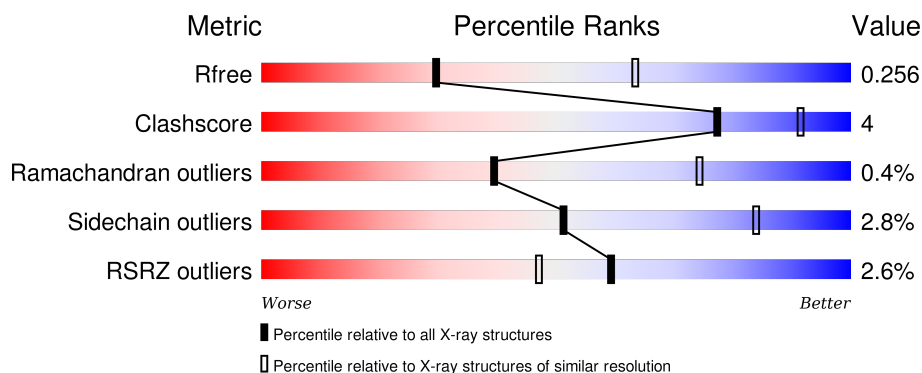
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	361	<div> <div>86%</div> <div>9% • 5%</div> </div>
1	B	361	<div> <div>79%</div> <div>15% 6%</div> </div>
1	C	361	<div> <div>83%</div> <div>11% • 6%</div> </div>
1	D	361	<div> <div>81%</div> <div>9% • 9%</div> </div>

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	1PE	A	502	-	-	-	X
3	1PE	A	503	-	-	-	X
4	SO4	B	504	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11273 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.

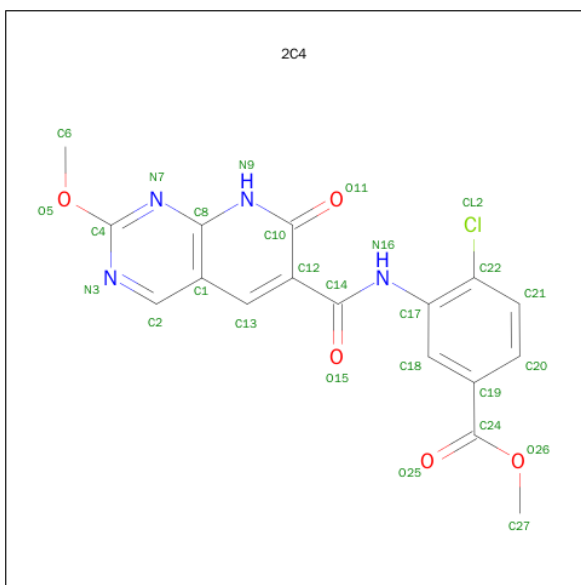
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	P	S	0	0	0
			2800	1800	480	502	1	17			
1	B	339	Total	C	N	O	P	S	0	0	0
			2752	1773	468	493	1	17			
1	C	340	Total	C	N	O	P	S	0	0	0
			2712	1750	457	488	1	16			
1	D	330	Total	C	N	O	P	S	0	1	0
			2662	1722	445	477	1	17			

There are 8 discrepancies between the modelled and reference sequences:

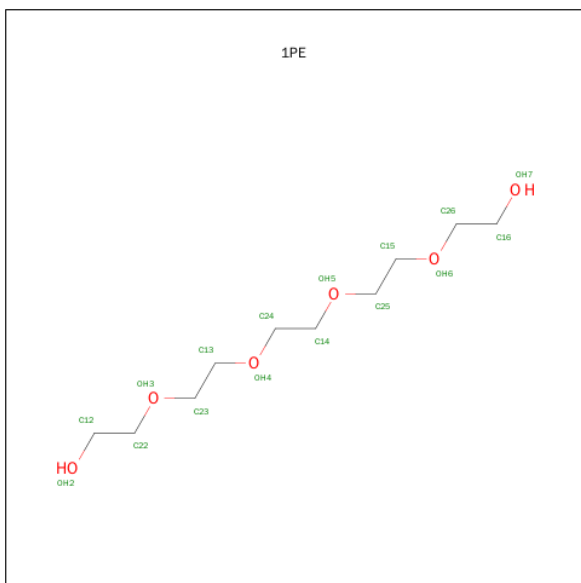
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	EXPRESSION TAG	UNP Q13627
A	126	MET	-	EXPRESSION TAG	UNP Q13627
B	125	SER	-	EXPRESSION TAG	UNP Q13627
B	126	MET	-	EXPRESSION TAG	UNP Q13627
C	125	SER	-	EXPRESSION TAG	UNP Q13627
C	126	MET	-	EXPRESSION TAG	UNP Q13627
D	125	SER	-	EXPRESSION TAG	UNP Q13627
D	126	MET	-	EXPRESSION TAG	UNP Q13627

- Molecule 2 is METHYL 4-CHLORO-3-[[[(2-METHOXY-7-OXO-7,8-DIHYDROPYRIDO[2,3-D]PYRIMIDIN-6-YL)CARBONYL]AMINO}BENZOATE (three-letter code: 2C4) (formula: C<sub>17</sub>H<sub>13</sub>ClN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 17	Cl 1	N 4	O 5	0	0
2	B	1	Total 27	C 17	Cl 1	N 4	O 5	0	0
2	C	1	Total 27	C 17	Cl 1	N 4	O 5	0	0
2	D	1	Total 27	C 17	Cl 1	N 4	O 5	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $\text{C}_{10}\text{H}_{22}\text{O}_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

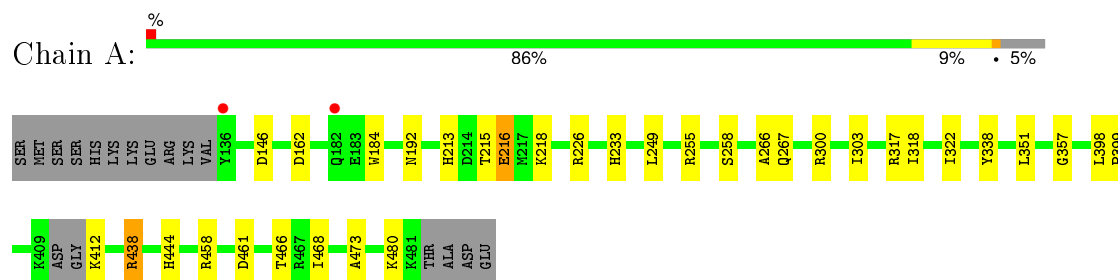
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	33	Total 33	O 33	0	0
5	C	16	Total 16	O 16	0	0
5	D	19	Total 19	O 19	0	0

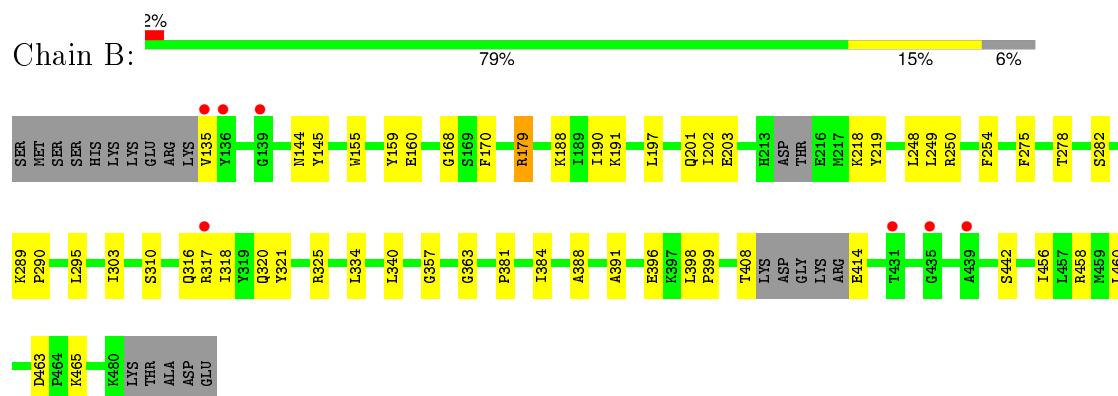
### 3 Residue-property plots [i](#)

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.

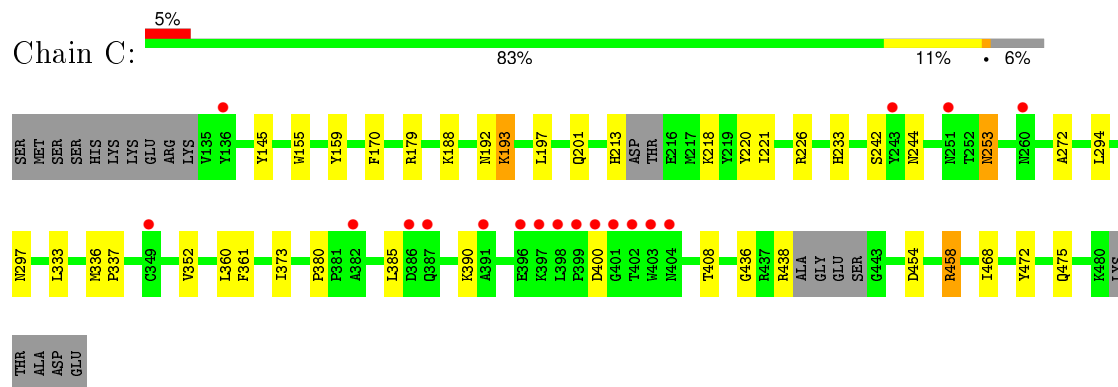
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



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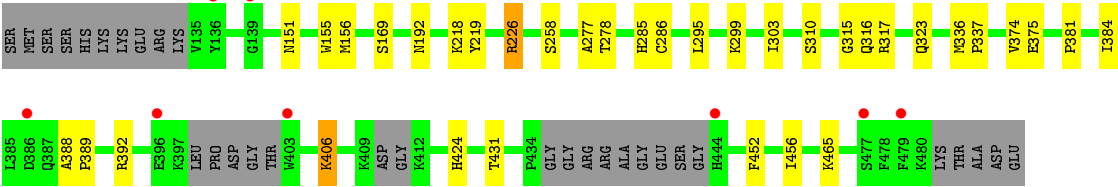
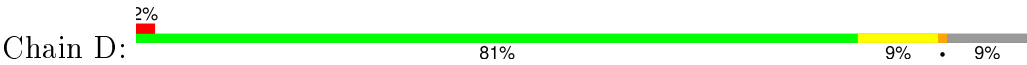


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.10Å 65.16Å 138.43Å 90.00° 115.01° 90.00°	Depositor
Resolution (Å)	36.78 – 2.80 36.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.78-2.80) 100.0 (36.30-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.190 , 0.258 0.194 , 0.256	Depositor DCC
$R_{free}$ test set	2652 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53114 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: 2C4, 1PE, PTR, SO4

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	0.71	0/2848	0.84	1/3842 (0.0%)
1	B	0.63	0/2799	0.79	2/3778 (0.1%)
1	C	0.59	0/2759	0.76	1/3733 (0.0%)
1	D	0.58	0/2710	0.74	2/3666 (0.1%)
All	All	0.63	0/11116	0.78	6/15019 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	458	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	458	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	B	463	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	226[A]	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	226[B]	ARG	NE-CZ-NH2	-5.32	117.64	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	LYS	Peptide
1	B	316	GLN	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	2800	0	2778	17	0
1	B	2752	0	2725	25	0
1	C	2712	0	2636	19	0
1	D	2662	0	2597	20	0
2	A	27	0	13	2	0
2	B	27	0	13	0	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	32	0	44	1	0
3	B	29	0	39	0	0
3	C	16	0	22	0	0
3	D	16	0	22	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
5	A	53	0	0	0	0
5	B	33	0	0	0	0
5	C	16	0	0	1	0
5	D	19	0	0	2	0
All	All	11273	0	10915	81	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 4.

All (81) 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:317:ARG:CB	1:B:318:ILE:HG13	1.67	1.23
1:B:317:ARG:CB	1:B:318:ILE:CG1	2.41	0.98
1:D:151:ASN:HB3	5:D:609:HOH:O	1.82	0.80
1:A:213:HIS:O	1:A:218:LYS:HD3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:SER:HA	1:A:438:ARG:HH21	1.57	0.70
1:B:414:GLU:OE2	1:D:299:LYS:NZ	2.26	0.67
1:B:325:ARG:HD2	1:B:363:GLY:O	1.98	0.64
1:B:250:ARG:HG2	1:B:254:PHE:CZ	2.34	0.62
1:D:226[A]:ARG:NH2	1:D:226[A]:ARG:HG3	2.15	0.61
1:A:322:ILE:HD11	1:A:338:TYR:CZ	2.37	0.59
2:A:501:2C4:O15	2:A:501:2C4:H10	2.04	0.58
1:D:226[A]:ARG:HG3	1:D:226[A]:ARG:HH21	1.69	0.57
1:B:317:ARG:CB	1:B:318:ILE:HG12	2.35	0.56
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.41	0.56
1:A:322:ILE:CD1	1:A:338:TYR:CZ	2.89	0.56
1:A:192:ASN:HB2	1:A:233:HIS:CE1	2.42	0.55
1:D:226[A]:ARG:CG	1:D:226[A]:ARG:HH21	2.18	0.55
1:A:322:ILE:HD11	1:A:338:TYR:CE2	2.43	0.54
1:D:392:ARG:O	1:D:406:LYS:HE3	2.08	0.53
1:D:424:HIS:HB2	5:D:607:HOH:O	2.08	0.53
1:A:438:ARG:HG3	1:A:444:HIS:CD2	2.45	0.52
1:B:320:GLN:O	1:B:321:PTR:C	2.59	0.51
1:A:266:ALA:HB2	1:A:351:LEU:HD22	1.93	0.51
1:D:286:CYS:O	1:D:323:GLN:HA	2.11	0.50
1:A:213:HIS:O	1:A:218:LYS:CD	2.59	0.49
1:A:317:ARG:HD2	1:A:338:TYR:CZ	2.47	0.49
1:A:216:GLU:HG3	1:C:297:ASN:HD21	1.77	0.49
1:D:452:PHE:CE1	1:D:456:ILE:HD11	2.48	0.49
1:B:197:LEU:O	1:B:201:GLN:HG3	2.13	0.49
1:A:398:LEU:O	1:A:399:PRO:C	2.50	0.49
1:A:184:TRP:NE1	3:A:502:1PE:H252	2.28	0.48
1:B:188:LYS:NZ	1:B:203:GLU:OE1	2.47	0.48
1:B:381:PRO:HG2	1:B:384:ILE:HD12	1.95	0.48
1:C:472:TYR:HA	1:C:475:GLN:HG3	1.96	0.48
1:B:249:LEU:HD22	1:B:357:GLY:HA2	1.97	0.47
1:C:155:TRP:HB2	1:C:159:TYR:HB2	1.96	0.46
1:D:285:HIS:O	1:D:286:CYS:HB2	2.15	0.46
1:C:436:GLY:O	1:C:438:ARG:N	2.49	0.46
1:B:144:ASN:O	1:B:145:TYR:HB2	2.16	0.45
1:C:352:VAL:HG11	1:C:360:LEU:HD13	1.98	0.45
1:C:454:ASP:O	1:C:458:ARG:HG2	2.15	0.45
1:C:145:TYR:CE2	1:C:193:LYS:HD3	2.52	0.45
1:B:289:LYS:HB2	1:B:290:PRO:HD2	1.99	0.45
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.99	0.45
2:A:501:2C4:O11	2:A:501:2C4:N16	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:HG22	1:B:191:LYS:N	2.32	0.44
1:B:334:LEU:HB3	1:B:388:ALA:HB1	1.99	0.44
1:D:374:VAL:O	1:D:375:GLU:C	2.55	0.43
1:D:388:ALA:O	1:D:389:PRO:C	2.56	0.43
1:A:258:SER:CA	1:A:438:ARG:HH21	2.30	0.43
1:C:380:PRO:HG2	1:C:385:LEU:HD21	1.99	0.43
1:B:218:LYS:O	1:B:219:TYR:CB	2.67	0.43
1:C:220:TYR:HB3	1:C:272:ALA:HB2	2.01	0.43
1:C:170:PHE:CD1	1:C:188:LYS:HE3	2.53	0.43
1:B:456:ILE:O	1:B:460:LEU:HG	2.19	0.43
1:A:461:ASP:OD2	1:A:466:THR:OG1	2.30	0.42
1:C:244:ASN:HA	1:C:294:LEU:HA	2.00	0.42
1:B:295:LEU:HD23	1:B:303:ILE:HG22	2.00	0.42
1:B:155:TRP:HB2	1:B:159:TYR:HB2	2.01	0.42
1:C:192:ASN:HB2	1:C:233:HIS:CE1	2.55	0.42
1:C:213:HIS:C	1:C:218:LYS:HD3	2.40	0.42
1:B:275:PHE:O	1:B:278:THR:HG23	2.20	0.42
1:B:340:LEU:HD12	1:B:340:LEU:N	2.34	0.42
1:D:295:LEU:HD23	1:D:303:ILE:HG22	2.01	0.42
1:D:218:LYS:HE2	1:D:219:TYR:CE1	2.55	0.41
1:D:155:TRP:O	1:D:156:MET:C	2.58	0.41
1:A:249:LEU:HD22	1:A:357:GLY:HA2	2.03	0.41
1:C:333:LEU:O	1:C:390:LYS:HE2	2.20	0.41
1:C:226:ARG:HD3	5:C:601:HOH:O	2.19	0.41
1:C:458:ARG:HB3	1:C:468:ILE:HB	2.03	0.41
1:C:336:MET:HB3	1:C:337:PRO:HD2	2.03	0.41
1:B:388:ALA:HB3	1:B:391:ALA:HB2	2.01	0.41
1:D:277:ALA:O	1:D:278:THR:C	2.59	0.41
1:D:315:GLY:O	1:D:317:ARG:N	2.51	0.41
1:D:381:PRO:HB2	1:D:384:ILE:HD12	2.04	0.40
1:C:197:LEU:O	1:C:201:GLN:HG3	2.21	0.40
1:D:192:ASN:OD1	1:D:192:ASN:O	2.39	0.40
1:B:160:GLU:OE1	1:B:179:ARG:HD3	2.22	0.40
1:B:168:GLY:HA3	1:B:170:PHE:CE1	2.56	0.40
1:D:336:MET:HB3	1:D:337:PRO:HD2	2.04	0.40
1:A:468:ILE:HD11	1:A:473:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

## 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	339/361 (94%)	311 (92%)	28 (8%)	0	100	100
1	B	332/361 (92%)	305 (92%)	27 (8%)	0	100	100
1	C	333/361 (92%)	304 (91%)	27 (8%)	2 (1%)	30	65
1	D	322/361 (89%)	289 (90%)	30 (9%)	3 (1%)	21	55
All	All	1326/1444 (92%)	1209 (91%)	112 (8%)	5 (0%)	39	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	ASN
1	C	400	ASP
1	D	258	SER
1	D	316	GLN
1	D	406	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	299/320 (93%)	287 (96%)	12 (4%)	38	73
1	B	294/320 (92%)	284 (97%)	10 (3%)	44	78
1	C	283/320 (88%)	277 (98%)	6 (2%)	61	90
1	D	281/320 (88%)	277 (99%)	4 (1%)	74	94
All	All	1157/1280 (90%)	1125 (97%)	32 (3%)	51	84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	A	162	ASP
1	A	215	THR
1	A	216	GLU
1	A	226	ARG
1	A	255	ARG
1	A	267	GLN
1	A	300	ARG
1	A	303	ILE
1	A	318	ILE
1	A	412	LYS
1	A	438	ARG
1	B	135	VAL
1	B	179	ARG
1	B	202	ILE
1	B	248	LEU
1	B	282	SER
1	B	310	SER
1	B	396	GLU
1	B	408	THR
1	B	442	SER
1	B	465	LYS
1	C	179	ARG
1	C	193	LYS
1	C	221	ILE
1	C	242	SER
1	C	253	ASN
1	C	408	THR
1	D	169	SER
1	D	310	SER
1	D	431	THR
1	D	465	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	B	267	GLN
1	B	425	ASN
1	C	469	GLN
1	D	137	ASN

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Mol	Chain	Res	Type
1	D	404	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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$
1	PTR	A	321	1	14,16,17	0.94	0	18,22,24	1.38	2 (11%)
1	PTR	B	321	1	14,16,17	1.12	1 (7%)	18,22,24	1.64	3 (16%)
1	PTR	C	321	1	14,16,17	0.70	0	18,22,24	1.09	1 (5%)
1	PTR	D	321	1	14,16,17	0.83	0	18,22,24	1.04	1 (5%)

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
1	PTR	A	321	1	-	0/9/11/13	0/1/1/1
1	PTR	B	321	1	-	0/9/11/13	0/1/1/1
1	PTR	C	321	1	-	0/9/11/13	0/1/1/1
1	PTR	D	321	1	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PTR	CE2-CD2	2.06	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	CE2-CZ-CE1	-3.29	114.86	120.20
1	A	321	PTR	O2P-P-O1P	2.30	117.98	110.58
1	A	321	PTR	P-OH-CZ	2.32	130.44	123.76
1	D	321	PTR	O3P-P-O1P	2.34	118.10	110.58
1	C	321	PTR	O3P-P-O2P	2.43	116.63	107.38
1	B	321	PTR	CD2-CE2-CZ	2.67	123.11	119.74
1	B	321	PTR	P-OH-CZ	3.26	133.14	123.76

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
1	B	321	PTR	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

15 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	2C4	A	501	-	29,29,29	2.30	7 (24%)	32,41,41	2.78	11 (34%)
3	1PE	A	502	-	15,15,15	0.84	0	14,14,14	0.49	0
3	1PE	A	503	-	15,15,15	0.90	0	14,14,14	0.58	0
4	SO4	A	504	-	4,4,4	0.73	0	6,6,6	1.20	1 (16%)
4	SO4	A	505	-	4,4,4	0.51	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2C4	B	501	-	29,29,29	2.33	8 (27%)	32,41,41	2.53	9 (28%)
3	1PE	B	502	-	15,15,15	0.93	0	14,14,14	0.58	0
3	1PE	B	503	-	12,12,15	0.82	0	11,11,14	0.58	0
4	SO4	B	504	-	4,4,4	0.62	0	6,6,6	0.39	0
4	SO4	B	505	-	4,4,4	0.52	0	6,6,6	0.62	0
4	SO4	B	506	-	4,4,4	0.60	0	6,6,6	0.27	0
2	2C4	C	501	-	29,29,29	2.28	7 (24%)	32,41,41	2.71	14 (43%)
3	1PE	C	502	-	15,15,15	0.94	0	14,14,14	0.50	0
2	2C4	D	501	-	29,29,29	2.06	9 (31%)	32,41,41	2.88	14 (43%)
3	1PE	D	502	-	15,15,15	0.72	0	14,14,14	0.78	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	2C4	A	501	-	-	0/16/16/16	0/3/3/3
3	1PE	A	502	-	-	0/13/13/13	0/0/0/0
3	1PE	A	503	-	-	0/13/13/13	0/0/0/0
4	SO4	A	504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	2C4	B	501	-	-	0/16/16/16	0/3/3/3
3	1PE	B	502	-	-	0/13/13/13	0/0/0/0
3	1PE	B	503	-	-	0/10/10/13	0/0/0/0
4	SO4	B	504	-	-	0/0/0/0	0/0/0/0
4	SO4	B	505	-	-	0/0/0/0	0/0/0/0
4	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	2C4	C	501	-	-	0/16/16/16	0/3/3/3
3	1PE	C	502	-	-	0/13/13/13	0/0/0/0
2	2C4	D	501	-	-	0/16/16/16	0/3/3/3
3	1PE	D	502	-	-	0/13/13/13	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	2C4	C12-C14	-6.72	1.39	1.50
2	C	501	2C4	C12-C14	-6.08	1.40	1.50
2	A	501	2C4	C12-C14	-5.74	1.41	1.50
2	D	501	2C4	C12-C14	-4.79	1.42	1.50
2	A	501	2C4	C17-N16	-4.25	1.33	1.41
2	C	501	2C4	C19-C24	-4.20	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2C4	C19-C24	-4.10	1.40	1.49
2	B	501	2C4	C19-C24	-4.06	1.40	1.49
2	B	501	2C4	C17-N16	-3.22	1.35	1.41
2	D	501	2C4	C19-C24	-2.84	1.43	1.49
2	C	501	2C4	C17-N16	-2.59	1.36	1.41
2	D	501	2C4	C17-N16	-2.53	1.37	1.41
2	D	501	2C4	C8-N7	-2.46	1.32	1.36
2	B	501	2C4	C4-N7	2.11	1.36	1.33
2	D	501	2C4	C18-C17	2.12	1.42	1.39
2	B	501	2C4	C4-N3	2.14	1.35	1.33
2	D	501	2C4	C22-CL2	2.14	1.78	1.73
2	D	501	2C4	C13-C12	2.31	1.41	1.37
2	C	501	2C4	C13-C12	2.33	1.41	1.37
2	B	501	2C4	C8-N9	2.56	1.40	1.34
2	C	501	2C4	C8-N9	2.68	1.40	1.34
2	A	501	2C4	C8-N9	2.79	1.40	1.34
2	A	501	2C4	C4-N7	2.96	1.37	1.33
2	B	501	2C4	C10-N9	4.31	1.41	1.33
2	A	501	2C4	C10-N9	4.44	1.41	1.33
2	D	501	2C4	C2-N3	4.51	1.39	1.32
2	C	501	2C4	C2-N3	4.76	1.40	1.32
2	D	501	2C4	C10-N9	5.36	1.43	1.33
2	A	501	2C4	C2-N3	5.58	1.41	1.32
2	B	501	2C4	C2-N3	5.73	1.41	1.32
2	C	501	2C4	C10-N9	5.99	1.44	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C4	N3-C4-N7	-11.45	121.03	128.33
2	C	501	2C4	N3-C4-N7	-10.77	121.46	128.33
2	B	501	2C4	N3-C4-N7	-9.88	122.03	128.33
2	A	501	2C4	N3-C4-N7	-9.84	122.06	128.33
2	A	501	2C4	C1-C8-N9	-5.33	117.16	122.52
2	B	501	2C4	C1-C8-N9	-4.99	117.50	122.52
2	C	501	2C4	C27-O26-C24	-4.58	106.43	115.84
2	A	501	2C4	C22-C17-N16	-4.27	111.90	119.37
2	A	501	2C4	C6-O5-C4	-4.11	109.95	117.63
2	D	501	2C4	C27-O26-C24	-3.60	108.44	115.84
2	D	501	2C4	C22-C17-N16	-3.55	113.16	119.37
2	D	501	2C4	O15-C14-C12	-3.37	116.64	121.59
2	B	501	2C4	C22-C17-N16	-3.15	113.86	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	2C4	C1-C2-N3	-2.95	118.64	124.06
2	C	501	2C4	C22-C17-N16	-2.94	114.23	119.37
2	D	501	2C4	C20-C19-C18	-2.90	115.73	119.24
2	D	501	2C4	C1-C8-N7	-2.79	119.70	122.50
2	C	501	2C4	C1-C2-N3	-2.77	118.98	124.06
2	D	501	2C4	C6-O5-C4	-2.77	112.46	117.63
2	B	501	2C4	O15-C14-C12	-2.74	117.57	121.59
2	D	501	2C4	C1-C2-N3	-2.64	119.22	124.06
2	B	501	2C4	C1-C2-N3	-2.62	119.25	124.06
2	C	501	2C4	C1-C8-N9	-2.52	119.99	122.52
2	C	501	2C4	O15-C14-C12	-2.32	118.18	121.59
2	A	501	2C4	C17-N16-C14	-2.30	120.66	127.06
2	C	501	2C4	C1-C8-N7	-2.18	120.31	122.50
2	C	501	2C4	C20-C19-C24	-2.09	115.68	120.39
2	B	501	2C4	C6-O5-C4	-2.03	113.84	117.63
2	A	501	2C4	C18-C17-N16	2.08	127.47	122.00
2	B	501	2C4	C18-C17-N16	2.10	127.52	122.00
2	C	501	2C4	C18-C19-C24	2.11	124.24	120.11
2	A	501	2C4	O5-C4-N7	2.23	123.77	116.26
2	D	501	2C4	C18-C19-C24	2.23	124.48	120.11
2	C	501	2C4	C18-C17-N16	2.29	128.02	122.00
2	A	501	2C4	C18-C17-C22	2.30	120.51	118.08
2	D	501	2C4	C12-C14-N16	2.48	118.62	114.67
2	D	501	2C4	C18-C17-N16	2.54	128.69	122.00
4	A	504	SO4	O2-S-O1	2.57	117.64	109.50
2	C	501	2C4	C17-C22-CL2	2.65	122.93	119.45
2	D	501	2C4	N7-C8-N9	2.75	119.53	116.03
2	C	501	2C4	O26-C24-C19	2.79	117.09	112.36
2	C	501	2C4	N7-C8-N9	2.88	119.70	116.03
2	D	501	2C4	O26-C24-C19	2.93	117.33	112.36
2	D	501	2C4	C2-N3-C4	3.64	119.09	115.06
2	B	501	2C4	C2-N3-C4	3.77	119.24	115.06
2	B	501	2C4	N7-C8-N9	3.81	120.89	116.03
2	C	501	2C4	C2-N3-C4	3.93	119.41	115.06
2	A	501	2C4	C2-N3-C4	4.25	119.77	115.06
2	A	501	2C4	N7-C8-N9	4.93	122.32	116.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	2C4	2	0
3	A	502	1PE	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	343/361 (95%)	-0.30	2 (0%) 90 86	25, 40, 70, 88	0
1	B	338/361 (93%)	-0.13	7 (2%) 67 56	28, 46, 76, 118	0
1	C	339/361 (93%)	-0.05	18 (5%) 30 20	39, 62, 94, 115	0
1	D	329/361 (91%)	-0.13	8 (2%) 62 50	35, 59, 90, 114	0
All	All	1349/1444 (93%)	-0.15	35 (2%) 59 47	25, 52, 86, 118	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	402	THR	5.2
1	B	135	VAL	4.5
1	C	403	TRP	3.9
1	C	399	PRO	3.6
1	B	136	TYR	3.4
1	C	404	ASN	3.4
1	C	401	GLY	3.3
1	C	398	LEU	3.2
1	C	382	ALA	3.0
1	C	387	GLN	3.0
1	C	386	ASP	2.8
1	D	386	ASP	2.8
1	C	400	ASP	2.8
1	D	403	TRP	2.7
1	D	396	GLU	2.7
1	B	439	ALA	2.7
1	C	397	LYS	2.7
1	A	136	TYR	2.6
1	D	136	TYR	2.5
1	A	182	GLN	2.4
1	D	479	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	136	TYR	2.4
1	B	431	THR	2.4
1	C	260	ASN	2.3
1	B	317	ARG	2.3
1	B	139	GLY	2.3
1	C	391	ALA	2.1
1	C	349	CYS	2.1
1	C	251	ASN	2.1
1	D	477	SER	2.1
1	D	139	GLY	2.0
1	D	444	HIS	2.0
1	C	243	TYR	2.0
1	B	435	GLY	2.0
1	C	396	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	C	321	16/17	0.92	0.15	-	59,69,82,84	0
1	PTR	D	321	16/17	0.93	0.19	-	61,77,85,88	0
1	PTR	A	321	16/17	0.97	0.15	-	34,38,51,54	0
1	PTR	B	321	16/17	0.92	0.28	-	64,72,80,82	0

## 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
3	1PE	A	503	16/16	0.95	0.20	3.01	37,46,54,58	0
4	SO4	B	504	5/5	0.95	0.24	2.80	55,57,74,75	0
3	1PE	A	502	16/16	0.94	0.24	2.18	64,68,74,76	0
4	SO4	A	504	5/5	0.95	0.21	1.66	53,62,70,71	0
4	SO4	A	505	5/5	0.75	0.27	1.32	97,107,108,126	0
3	1PE	C	502	16/16	0.91	0.22	0.42	64,68,79,83	0
3	1PE	B	503	13/16	0.96	0.16	0.38	32,38,45,47	0
3	1PE	B	502	16/16	0.92	0.20	0.19	63,70,78,79	0
2	2C4	D	501	27/27	0.96	0.14	-0.27	41,46,53,54	0
2	2C4	C	501	27/27	0.96	0.13	-0.59	51,59,66,70	0
2	2C4	B	501	27/27	0.96	0.16	-0.62	32,37,46,50	0
2	2C4	A	501	27/27	0.97	0.13	-0.92	34,37,46,48	0
3	1PE	D	502	16/16	0.97	0.11	-1.33	39,45,52,54	0
4	SO4	B	506	5/5	0.97	0.21	-	62,62,70,73	0
4	SO4	B	505	5/5	0.90	0.25	-	82,88,100,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.