



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:47 PM GMT

PDB ID : 4MQ1
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 : 2.35 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

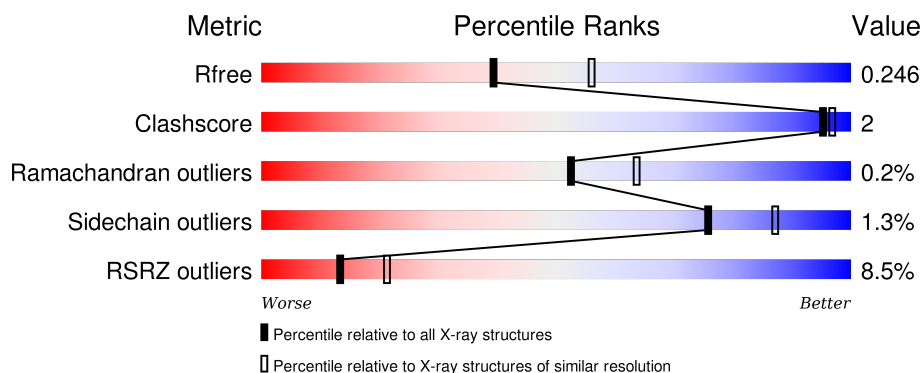
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	<div> <div>7%</div> <div>92%</div> <div>• •</div> </div>
1	B	361	<div> <div>7%</div> <div>87%</div> <div>7% 6%</div> </div>
1	C	361	<div> <div>12%</div> <div>86%</div> <div>5% 9%</div> </div>
1	D	361	<div> <div>6%</div> <div>87%</div> <div>6% • 7%</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	D	504	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11696 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.

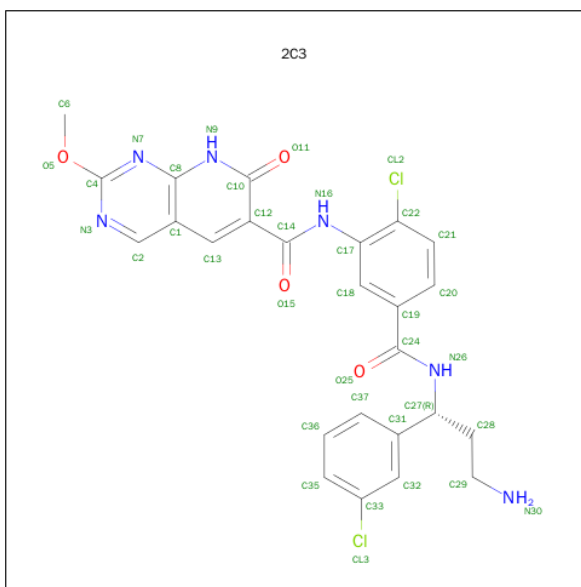
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	P	S	0	1	0
			2829	1818	482	510	2	17			
1	B	341	Total	C	N	O	P	S	0	0	0
			2771	1784	471	498	1	17			
1	C	329	Total	C	N	O	P	S	0	0	0
			2635	1704	438	476	1	16			
1	D	337	Total	C	N	O	P	S	0	1	0
			2710	1746	463	483	1	17			

There are 8 discrepancies between the modelled and reference sequences:

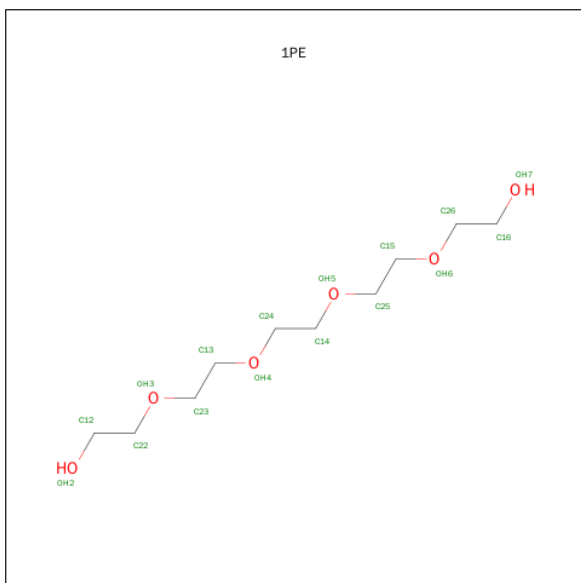
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	-	EXPRESSION TAG	UNP Q13627
A	126	MET	-	EXPRESSION TAG	UNP Q13627
B	125	SER	-	EXPRESSION TAG	UNP Q13627
B	126	MET	-	EXPRESSION TAG	UNP Q13627
C	125	SER	-	EXPRESSION TAG	UNP Q13627
C	126	MET	-	EXPRESSION TAG	UNP Q13627
D	125	SER	-	EXPRESSION TAG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

- Molecule 2 is N-(5-([(1R)-3-AMINO-1-(3-CHLOROPHENYL)PROPYL]CARBAMOYL})-2-CHLOROPHENYL)-2-METHOXY-7-OXO-7,8-DIHYDROPYRIDO[2,3-D]PYRIMIDINE-6-CARBOXAMIDE (three-letter code: 2C3) (formula: C₂₅H₂₂Cl₂N₆O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 37	C 25	Cl 2	N 6	O 4	0	0
2	B	1	Total 37	C 25	Cl 2	N 6	O 4	0	0
2	C	1	Total 37	C 25	Cl 2	N 6	O 4	0	0
2	D	1	Total 37	C 25	Cl 2	N 6	O 4	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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: O₄S).



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	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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

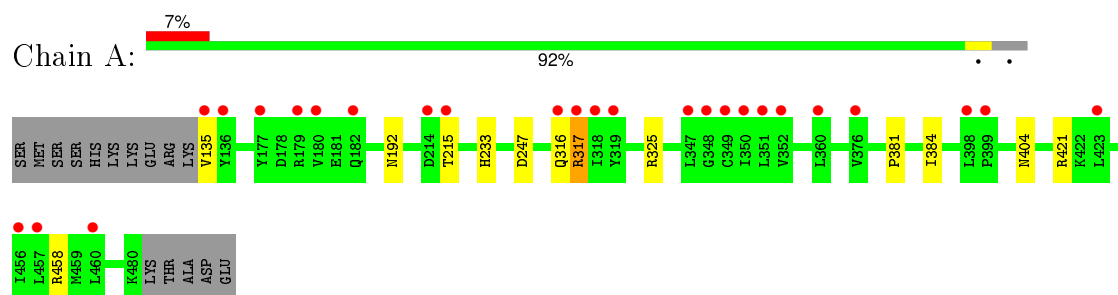
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	162	Total	O	0	0
			162	162		
5	C	50	Total	O	0	0
			50	50		
5	D	55	Total	O	0	0
			55	55		

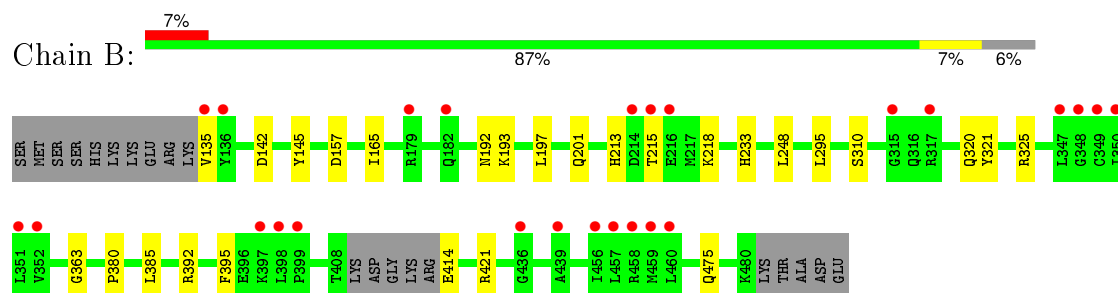
3 Residue-property plots [i](#)

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.

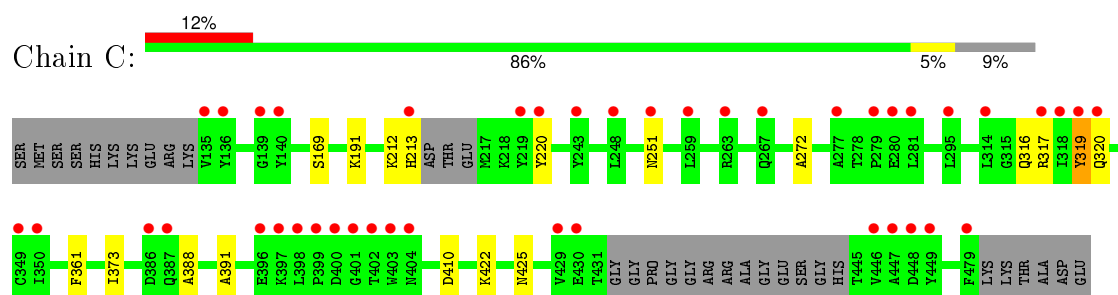
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



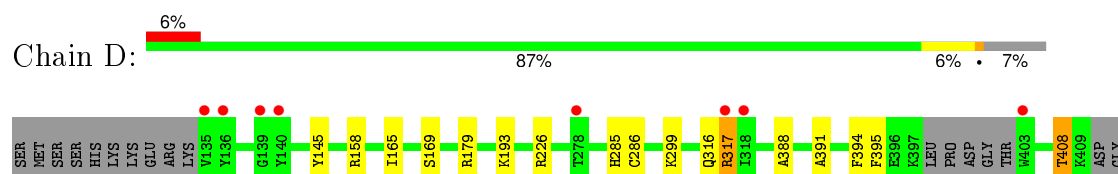
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

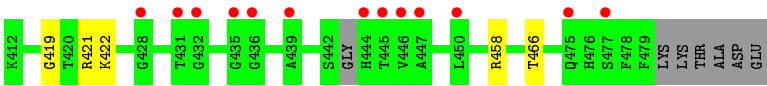


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- 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, α , β , γ	263.84Å 64.94Å 140.46Å 90.00° 115.16° 90.00°	Depositor
Resolution (Å)	39.83 – 2.35 39.44 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.83-2.35) 99.7 (39.44-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.246 0.205 , 0.246	Depositor DCC
R_{free} test set	4498 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90011 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11696	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 2C3, PTR, 1PE

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	0.68	0/2862	0.79	6/3862 (0.2%)
1	B	0.61	0/2819	0.74	2/3806 (0.1%)
1	C	0.51	0/2679	0.67	1/3628 (0.0%)
1	D	0.54	0/2757	0.70	1/3725 (0.0%)
All	All	0.59	0/11117	0.73	10/15021 (0.1%)

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	C	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	458	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	247	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	325	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	142	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	325	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	421	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	421	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	320	GLN	N-CA-C	-5.06	97.33	111.00
1	B	421	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	319	TYR	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	2829	0	2803	4	0
1	B	2771	0	2748	11	0
1	C	2635	0	2561	6	0
1	D	2710	0	2653	13	0
2	A	37	0	22	1	0
2	B	37	0	22	1	0
2	C	37	0	22	1	0
2	D	37	0	22	1	0
3	A	32	0	44	0	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	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	203	0	0	0	0
5	B	162	0	0	0	0
5	C	50	0	0	0	0
5	D	55	0	0	2	0
All	All	11696	0	10980	35	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 2.

All (35) 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:192:ASN:HB2	1:A:233:HIS:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ARG:HD2	1:B:363:GLY:O	1.99	0.62
1:A:316:GLN:O	1:A:317:ARG:O	2.24	0.56
1:D:408:THR:HG23	5:D:655:HOH:O	2.07	0.55
2:A:501:2C3:O15	2:A:501:2C3:H12	2.07	0.54
1:B:320:GLN:O	1:B:321:PTR:C	2.58	0.51
1:D:316:GLN:O	1:D:317:ARG:O	2.29	0.49
1:D:226[B]:ARG:NH2	5:D:601:HOH:O	2.42	0.49
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.94	0.49
1:C:169:SER:O	1:C:191:LYS:HE3	2.12	0.49
1:D:165:ILE:O	1:D:165:ILE:HG22	2.12	0.48
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.96	0.47
1:C:316:GLN:O	1:C:317:ARG:C	2.53	0.47
1:B:165:ILE:HG21	2:B:501:2C3:C13	2.46	0.46
1:A:381:PRO:HG2	1:A:384:ILE:HD12	1.98	0.46
1:D:285:HIS:O	1:D:286:CYS:HB2	2.17	0.45
1:D:158:ARG:O	1:D:179:ARG:HG3	2.17	0.45
1:B:414:GLU:OE1	1:D:299:LYS:NZ	2.44	0.45
1:A:316:GLN:O	1:A:317:ARG:C	2.56	0.45
1:D:145:TYR:CE1	1:D:193:LYS:HD3	2.53	0.44
1:B:145:TYR:CE1	1:B:193:LYS:HD2	2.53	0.43
1:B:248:LEU:HD21	1:B:295:LEU:HD11	2.01	0.43
1:B:213:HIS:O	1:B:218:LYS:HD3	2.19	0.43
2:C:501:2C3:C37	2:C:501:2C3:C29	2.97	0.42
1:B:392:ARG:HA	1:B:395:PHE:O	2.19	0.42
1:B:197:LEU:O	1:B:201:GLN:HG3	2.19	0.42
1:D:394:PHE:HB2	1:D:395:PHE:CD2	2.54	0.42
1:C:422:LYS:HB2	1:C:425:ASN:HD22	1.85	0.42
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.55	0.41
1:D:165:ILE:HG21	2:D:501:2C3:C13	2.51	0.41
1:B:380:PRO:HG2	1:B:385:LEU:HD21	2.03	0.41
1:D:458:ARG:NH1	1:D:466:THR:O	2.43	0.41
1:D:419:GLY:O	1:D:422:LYS:HE3	2.21	0.41
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.56	0.40
1:C:220:TYR:HB3	1:C:272:ALA:HB2	2.04	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	343/361 (95%)	320 (93%)	22 (6%)	1 (0%)	46	55
1	B	336/361 (93%)	326 (97%)	10 (3%)	0	100	100
1	C	322/361 (89%)	305 (95%)	17 (5%)	0	100	100
1	D	329/361 (91%)	308 (94%)	20 (6%)	1 (0%)	46	55
All	All	1330/1444 (92%)	1259 (95%)	69 (5%)	2 (0%)	52	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ARG
1	D	317	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/320 (94%)	298 (99%)	3 (1%)	82	91
1	B	297/320 (93%)	292 (98%)	5 (2%)	68	82
1	C	277/320 (87%)	272 (98%)	5 (2%)	66	81
1	D	284/320 (89%)	282 (99%)	2 (1%)	88	95
All	All	1159/1280 (90%)	1144 (99%)	15 (1%)	76	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	215	THR
1	A	404	ASN
1	B	135	VAL
1	B	157	ASP
1	B	215	THR
1	B	310	SER
1	B	475	GLN
1	C	212	LYS
1	C	213	HIS
1	C	251	ASN
1	C	319	TYR
1	C	410	ASP
1	D	169	SER
1	D	408	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	383	HIS
1	B	404	ASN
1	B	425	ASN
1	C	198	ASN
1	C	253	ASN
1	C	404	ASN
1	C	425	ASN
1	C	469	GLN
1	D	198	ASN
1	D	404	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](#)

5 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[A]	1	14,16,17	0.78	0	18,22,24	1.69	3 (16%)
1	PTR	A	321[B]	1	14,16,17	1.02	1 (7%)	18,22,24	1.54	3 (16%)
1	PTR	B	321	1	14,16,17	1.27	2 (14%)	18,22,24	1.43	4 (22%)
1	PTR	C	321	1	14,16,17	0.68	0	18,22,24	1.47	3 (16%)
1	PTR	D	321	1	14,16,17	0.84	0	18,22,24	1.88	5 (27%)

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[A]	1	-	0/9/11/13	0/1/1/1
1	PTR	A	321[B]	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321[B]	PTR	CE1-CD1	2.01	1.42	1.38
1	B	321	PTR	CE2-CZ	2.06	1.42	1.38
1	B	321	PTR	CE2-CD2	2.46	1.43	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321[A]	PTR	CG-CB-CA	-5.03	102.85	114.21
1	D	321	PTR	CG-CB-CA	-4.59	103.83	114.21
1	D	321	PTR	P-OH-CZ	-3.06	114.96	123.76
1	C	321	PTR	O2P-P-OH	-2.51	96.22	105.22
1	A	321[B]	PTR	CE2-CZ-CE1	-2.38	116.34	120.20
1	A	321[A]	PTR	CB-CG-CD2	-2.24	116.20	120.90
1	B	321	PTR	CE2-CZ-CE1	-2.10	116.80	120.20
1	B	321	PTR	OH-CZ-CE2	2.09	125.66	119.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	O3P-P-O1P	2.10	117.34	110.58
1	A	321[B]	PTR	OH-CZ-CE1	2.11	125.72	119.22
1	D	321	PTR	O3P-P-O1P	2.11	117.37	110.58
1	D	321	PTR	CD2-CG-CD1	2.43	122.03	118.13
1	D	321	PTR	O3P-P-O2P	2.95	118.61	107.38
1	C	321	PTR	O3P-P-O2P	2.96	118.65	107.38
1	A	321[A]	PTR	O3P-P-O2P	3.03	118.91	107.38
1	B	321	PTR	P-OH-CZ	3.60	134.10	123.76
1	A	321[B]	PTR	P-OH-CZ	3.76	134.57	123.76
1	C	321	PTR	CG-CB-CA	3.79	122.76	114.21

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 ⓘ

18 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	2C3	A	501	-	40,40,40	2.33	9 (22%)	44,56,56	2.64	10 (22%)
3	1PE	A	502	-	15,15,15	0.69	0	14,14,14	0.60	0
3	1PE	A	503	-	15,15,15	0.57	0	14,14,14	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	504	-	4,4,4	0.92	0	6,6,6	0.62	0
4	SO4	A	505	-	4,4,4	0.48	0	6,6,6	0.53	0
2	2C3	B	501	-	40,40,40	2.27	9 (22%)	44,56,56	2.31	10 (22%)
3	1PE	B	502	-	15,15,15	0.67	0	14,14,14	0.32	0
3	1PE	B	503	-	12,12,15	0.79	0	11,11,14	0.91	0
4	SO4	B	504	-	4,4,4	0.41	0	6,6,6	0.61	0
4	SO4	B	505	-	4,4,4	0.62	0	6,6,6	0.89	1 (16%)
2	2C3	C	501	-	40,40,40	2.32	10 (25%)	44,56,56	2.22	9 (20%)
3	1PE	C	502	-	15,15,15	0.77	0	14,14,14	0.48	0
4	SO4	C	503	-	4,4,4	0.34	0	6,6,6	0.37	0
4	SO4	C	504	-	4,4,4	0.74	0	6,6,6	0.17	0
2	2C3	D	501	-	40,40,40	2.33	10 (25%)	44,56,56	2.62	12 (27%)
3	1PE	D	502	-	15,15,15	0.55	0	14,14,14	0.70	0
4	SO4	D	503	-	4,4,4	0.55	0	6,6,6	0.25	0
4	SO4	D	504	-	4,4,4	0.64	0	6,6,6	0.76	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	2C3	A	501	-	-	0/25/25/25	0/4/4/4
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	2C3	B	501	-	-	0/25/25/25	0/4/4/4
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
2	2C3	C	501	-	-	0/25/25/25	0/4/4/4
3	1PE	C	502	-	-	0/13/13/13	0/0/0/0
4	SO4	C	503	-	-	0/0/0/0	0/0/0/0
4	SO4	C	504	-	-	0/0/0/0	0/0/0/0
2	2C3	D	501	-	-	0/25/25/25	0/4/4/4
3	1PE	D	502	-	-	0/13/13/13	0/0/0/0
4	SO4	D	503	-	-	0/0/0/0	0/0/0/0
4	SO4	D	504	-	-	0/0/0/0	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	2C3	C31-C27	-8.94	1.39	1.52
2	D	501	2C3	C31-C27	-8.73	1.39	1.52
2	B	501	2C3	C31-C27	-7.86	1.40	1.52
2	A	501	2C3	C31-C27	-7.48	1.41	1.52
2	B	501	2C3	C12-C14	-6.63	1.39	1.50
2	D	501	2C3	C12-C14	-5.38	1.41	1.50
2	A	501	2C3	C19-C24	-5.29	1.39	1.50
2	A	501	2C3	C12-C14	-5.06	1.42	1.50
2	B	501	2C3	C19-C24	-4.51	1.40	1.50
2	C	501	2C3	C12-C14	-4.16	1.43	1.50
2	C	501	2C3	C19-C24	-4.13	1.41	1.50
2	B	501	2C3	C33-CL3	-3.31	1.67	1.74
2	D	501	2C3	C19-C24	-3.26	1.43	1.50
2	C	501	2C3	C17-N16	-3.12	1.35	1.41
2	C	501	2C3	C33-CL3	-2.70	1.68	1.74
2	A	501	2C3	C17-N16	-2.68	1.36	1.41
2	B	501	2C3	C2-C1	-2.47	1.36	1.41
2	D	501	2C3	C17-N16	-2.45	1.37	1.41
2	D	501	2C3	C28-C27	-2.43	1.49	1.53
2	A	501	2C3	C33-CL3	-2.40	1.69	1.74
2	B	501	2C3	C17-N16	-2.39	1.37	1.41
2	B	501	2C3	C22-CL2	-2.04	1.68	1.73
2	C	501	2C3	C28-C27	-2.02	1.50	1.53
2	C	501	2C3	C4-N7	2.05	1.36	1.33
2	A	501	2C3	C27-N26	2.14	1.49	1.46
2	D	501	2C3	C4-N3	2.17	1.35	1.33
2	C	501	2C3	C8-N9	2.19	1.39	1.34
2	D	501	2C3	C8-N9	2.46	1.39	1.34
2	B	501	2C3	C10-N9	2.66	1.38	1.33
2	A	501	2C3	C4-N7	3.11	1.37	1.33
2	D	501	2C3	C22-CL2	3.17	1.81	1.73
2	D	501	2C3	C10-N9	3.96	1.40	1.33
2	B	501	2C3	C2-N3	4.23	1.39	1.32
2	C	501	2C3	C2-N3	4.67	1.40	1.32
2	A	501	2C3	C2-N3	4.89	1.40	1.32
2	C	501	2C3	C10-N9	4.99	1.42	1.33
2	D	501	2C3	C2-N3	5.47	1.41	1.32
2	A	501	2C3	C10-N9	6.00	1.44	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	2C3	N3-C4-N7	-13.64	119.63	128.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	2C3	N3-C4-N7	-10.97	121.33	128.33
2	C	501	2C3	N3-C4-N7	-10.77	121.46	128.33
2	B	501	2C3	N3-C4-N7	-10.51	121.62	128.33
2	A	501	2C3	C1-C8-N9	-6.18	116.31	122.52
2	A	501	2C3	C29-C28-C27	-5.15	100.42	113.83
2	A	501	2C3	C22-C17-N16	-3.82	112.68	119.37
2	B	501	2C3	C1-C8-N9	-3.54	118.96	122.52
2	B	501	2C3	C22-C17-N16	-3.47	113.30	119.37
2	C	501	2C3	C22-C17-N16	-3.13	113.89	119.37
2	B	501	2C3	C1-C2-N3	-3.13	118.32	124.06
2	A	501	2C3	C1-C2-N3	-3.11	118.35	124.06
2	D	501	2C3	O15-C14-C12	-3.01	117.16	121.59
2	D	501	2C3	C1-C2-N3	-2.97	118.61	124.06
2	C	501	2C3	C1-C8-N9	-2.92	119.58	122.52
2	B	501	2C3	O15-C14-C12	-2.91	117.31	121.59
2	D	501	2C3	C22-C17-N16	-2.77	114.53	119.37
2	D	501	2C3	C31-C27-N26	-2.71	106.18	111.81
2	C	501	2C3	C1-C2-N3	-2.63	119.24	124.06
2	C	501	2C3	C1-C8-N7	-2.60	119.89	122.50
2	D	501	2C3	C1-C8-N7	-2.56	119.93	122.50
2	C	501	2C3	C32-C31-C27	-2.54	116.77	120.08
2	D	501	2C3	C1-C8-N9	-2.48	120.03	122.52
2	B	501	2C3	C6-O5-C4	-2.18	113.57	117.63
4	B	505	SO4	O2-S-O1	-2.15	102.68	109.50
2	D	501	2C3	C20-C19-C18	-2.12	116.68	119.24
2	B	501	2C3	C17-C22-CL2	-2.05	116.76	119.45
2	B	501	2C3	O5-C4-N7	2.00	123.01	116.26
2	D	501	2C3	C19-C18-C17	2.09	123.72	119.75
2	B	501	2C3	N7-C8-N9	2.11	118.71	116.03
2	C	501	2C3	C18-C17-N16	2.13	127.61	122.00
2	D	501	2C3	C18-C17-N16	2.31	128.07	122.00
2	A	501	2C3	C18-C17-N16	2.45	128.45	122.00
2	A	501	2C3	C12-C14-N16	2.70	118.97	114.67
2	A	501	2C3	O5-C4-N7	2.88	125.97	116.26
2	D	501	2C3	N7-C8-N9	3.15	120.04	116.03
2	C	501	2C3	C2-N3-C4	3.50	118.93	115.06
2	C	501	2C3	N7-C8-N9	3.53	120.53	116.03
2	D	501	2C3	C2-N3-C4	4.74	120.31	115.06
2	A	501	2C3	N7-C8-N9	5.11	122.54	116.03
2	A	501	2C3	C2-N3-C4	5.15	120.77	115.06
2	B	501	2C3	C2-N3-C4	5.34	120.98	115.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	2C3	1	0
2	B	501	2C3	1	0
2	C	501	2C3	1	0
2	D	501	2C3	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, 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	345/361 (95%)	0.29	26 (7%)	17	26	25, 38, 70, 94	0
1	B	340/361 (94%)	0.28	25 (7%)	17	27	27, 40, 67, 99	0
1	C	328/361 (90%)	0.66	43 (13%)	5	8	40, 62, 96, 115	0
1	D	336/361 (93%)	0.25	21 (6%)	23	35	34, 54, 87, 117	0
All	All	1349/1444 (93%)	0.37	115 (8%)	13	21	25, 49, 86, 117	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	398	LEU	6.8
1	C	403	TRP	5.9
1	A	135	VAL	5.9
1	D	318	ILE	5.8
1	C	402	THR	5.8
1	C	399	PRO	5.1
1	C	401	GLY	5.0
1	C	213	HIS	5.0
1	B	215	THR	4.9
1	C	318	ILE	4.5
1	B	214	ASP	4.5
1	C	448	ASP	4.4
1	B	317	ARG	4.4
1	A	318	ILE	4.4
1	B	135	VAL	4.3
1	A	215	THR	4.2
1	C	136	TYR	4.1
1	C	397	LYS	4.1
1	D	136	TYR	3.9
1	D	445	THR	3.9
1	C	251	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	259	LEU	3.7
1	B	350	ILE	3.7
1	D	439	ALA	3.7
1	C	219	TYR	3.6
1	D	403	TRP	3.6
1	B	457	LEU	3.6
1	C	400	ASP	3.6
1	A	456	ILE	3.5
1	D	135	VAL	3.5
1	B	351	LEU	3.5
1	C	243	TYR	3.5
1	C	447	ALA	3.4
1	B	439	ALA	3.4
1	C	319	TYR	3.4
1	A	214	ASP	3.3
1	A	136	TYR	3.3
1	D	447	ALA	3.2
1	A	460	LEU	3.2
1	C	295	LEU	3.2
1	C	277	ALA	3.1
1	A	180	VAL	3.1
1	D	435	GLY	3.0
1	C	280	GLU	3.0
1	D	431	THR	3.0
1	A	347	LEU	2.9
1	A	457	LEU	2.9
1	D	432	GLY	2.9
1	C	349	CYS	2.9
1	C	479	PHE	2.9
1	B	179	ARG	2.8
1	C	317	ARG	2.8
1	A	350	ILE	2.8
1	D	450	LEU	2.8
1	C	135	VAL	2.8
1	D	444	HIS	2.8
1	B	347	LEU	2.7
1	D	436	GLY	2.7
1	C	404	ASN	2.7
1	B	456	ILE	2.7
1	C	396	GLU	2.7
1	B	216	GLU	2.6
1	C	263	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	139	GLY	2.6
1	D	475	GLN	2.6
1	C	430	GLU	2.6
1	D	446	VAL	2.6
1	A	349	CYS	2.6
1	B	399	PRO	2.5
1	B	398	LEU	2.5
1	C	248	LEU	2.5
1	D	477	SER	2.5
1	A	182	GLN	2.5
1	B	136	TYR	2.5
1	A	360	LEU	2.5
1	C	220	TYR	2.5
1	B	315	GLY	2.4
1	A	398	LEU	2.4
1	A	348	GLY	2.4
1	A	423	LEU	2.4
1	A	351	LEU	2.4
1	A	352	VAL	2.4
1	C	320	GLN	2.4
1	D	140	TYR	2.4
1	C	387	GLN	2.3
1	B	349	CYS	2.3
1	C	446	VAL	2.3
1	B	459	MET	2.3
1	C	267	GLN	2.3
1	A	399	PRO	2.3
1	C	140	TYR	2.3
1	C	386	ASP	2.3
1	C	429	VAL	2.3
1	C	449	TYR	2.2
1	A	316	GLN	2.2
1	A	319	TYR	2.2
1	B	348	GLY	2.2
1	C	281	LEU	2.2
1	B	397	LYS	2.2
1	B	436	GLY	2.2
1	A	177	TYR	2.2
1	D	317	ARG	2.1
1	A	317	ARG	2.1
1	B	460	LEU	2.1
1	C	314	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	350	ILE	2.1
1	A	376	VAL	2.1
1	B	182	GLN	2.1
1	A	179	ARG	2.0
1	C	279	PRO	2.0
1	B	458	ARG	2.0
1	D	278	THR	2.0
1	D	139	GLY	2.0
1	D	428	GLY	2.0
1	B	352	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	A	321[A]	16/17	0.89	0.19	-	28,33,47,53	16
1	PTR	B	321	16/17	0.95	0.15	-	42,54,57,59	0
1	PTR	D	321	16/17	0.93	0.16	-	55,73,85,88	0
1	PTR	C	321	16/17	0.91	0.17	-	52,73,84,84	0
1	PTR	A	321[B]	16/17	0.89	0.19	-	38,51,56,59	16

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	D	504	5/5	0.85	0.24	5.17	78,86,95,98	0
3	1PE	A	503	16/16	0.92	0.24	4.55	37,46,54,61	0
3	1PE	A	502	16/16	0.88	0.23	2.11	62,67,87,87	0
3	1PE	B	503	13/16	0.94	0.16	1.59	34,37,40,50	0
4	SO4	A	504	5/5	0.92	0.20	0.64	47,55,63,75	0
3	1PE	D	502	16/16	0.95	0.14	0.49	40,52,62,64	0
3	1PE	B	502	16/16	0.91	0.14	0.39	48,62,74,75	0
3	1PE	C	502	16/16	0.89	0.17	-0.03	66,71,80,81	0
2	2C3	C	501	37/37	0.94	0.12	-0.72	52,60,73,75	0
2	2C3	B	501	37/37	0.95	0.14	-0.73	30,35,43,51	0
4	SO4	C	503	5/5	0.97	0.12	-0.77	80,81,83,95	0
2	2C3	D	501	37/37	0.96	0.11	-0.91	36,44,56,56	0
2	2C3	A	501	37/37	0.95	0.11	-0.92	26,34,47,53	0
4	SO4	A	505	5/5	0.97	0.10	-1.11	50,55,61,61	0
4	SO4	D	503	5/5	0.97	0.09	-1.40	57,63,75,79	0
4	SO4	B	505	5/5	0.96	0.12	-2.50	42,51,65,71	0
4	SO4	B	504	5/5	0.98	0.11	-	56,59,63,65	0
4	SO4	C	504	5/5	0.88	0.27	-	74,87,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.