



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:46 PM UTC

PDB ID : 5XU6 / pdb_00005xu6
Title : Crystal structure of inositol 1,3,4,5,6-pentakisphosphate 2-kinase (IPK1) from *Cryptococcus neoformans*
Authors : Oh, J.; Rhee, S.
Deposited on : 2017-06-22
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

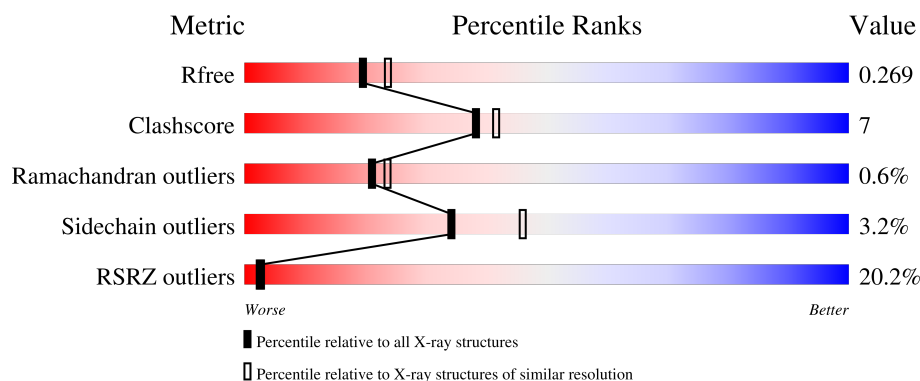
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	417	21% 74% 12% • 12%
1	B	417	21% 66% 17% • 15%
1	C	417	14% 72% 17% • 9%
1	D	417	15% 75% 13% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11782 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 Inositol-pentakisphosphate 2-kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	Se	0	0	0
			2802	1782	495	518	2	5			
1	B	354	Total	C	N	O	S	Se	0	0	0
			2676	1705	471	494	2	4			
1	C	379	Total	C	N	O	S	Se	0	0	0
			2960	1885	516	551	2	6			
1	D	377	Total	C	N	O	S	Se	0	0	0
			2942	1876	514	544	2	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP J9VKS8
A	0	HIS	-	expression tag	UNP J9VKS8
A	64	ALA	GLN	engineered mutation	UNP J9VKS8
A	66	ALA	GLU	engineered mutation	UNP J9VKS8
A	67	ALA	GLU	engineered mutation	UNP J9VKS8
B	-1	GLY	-	expression tag	UNP J9VKS8
B	0	HIS	-	expression tag	UNP J9VKS8
B	64	ALA	GLN	engineered mutation	UNP J9VKS8
B	66	ALA	GLU	engineered mutation	UNP J9VKS8
B	67	ALA	GLU	engineered mutation	UNP J9VKS8
C	-1	GLY	-	expression tag	UNP J9VKS8
C	0	HIS	-	expression tag	UNP J9VKS8
C	64	ALA	GLN	engineered mutation	UNP J9VKS8
C	66	ALA	GLU	engineered mutation	UNP J9VKS8
C	67	ALA	GLU	engineered mutation	UNP J9VKS8
D	-1	GLY	-	expression tag	UNP J9VKS8
D	0	HIS	-	expression tag	UNP J9VKS8
D	64	ALA	GLN	engineered mutation	UNP J9VKS8
D	66	ALA	GLU	engineered mutation	UNP J9VKS8
D	67	ALA	GLU	engineered mutation	UNP J9VKS8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	37	Total	O	0	0
			37	37		

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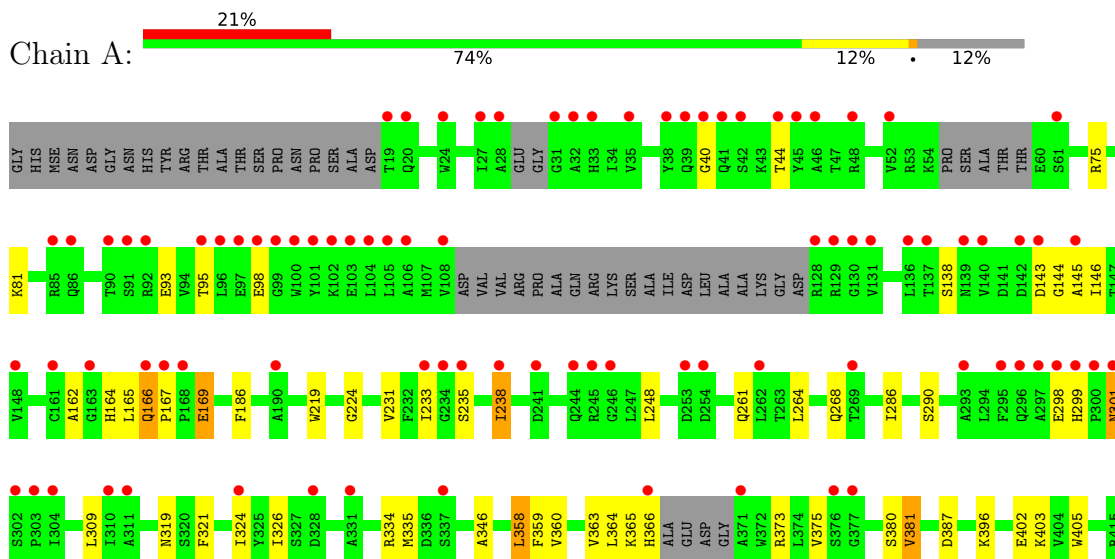
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	149	Total	O	0	0
			149	149		
3	D	96	Total	O	0	0
			96	96		

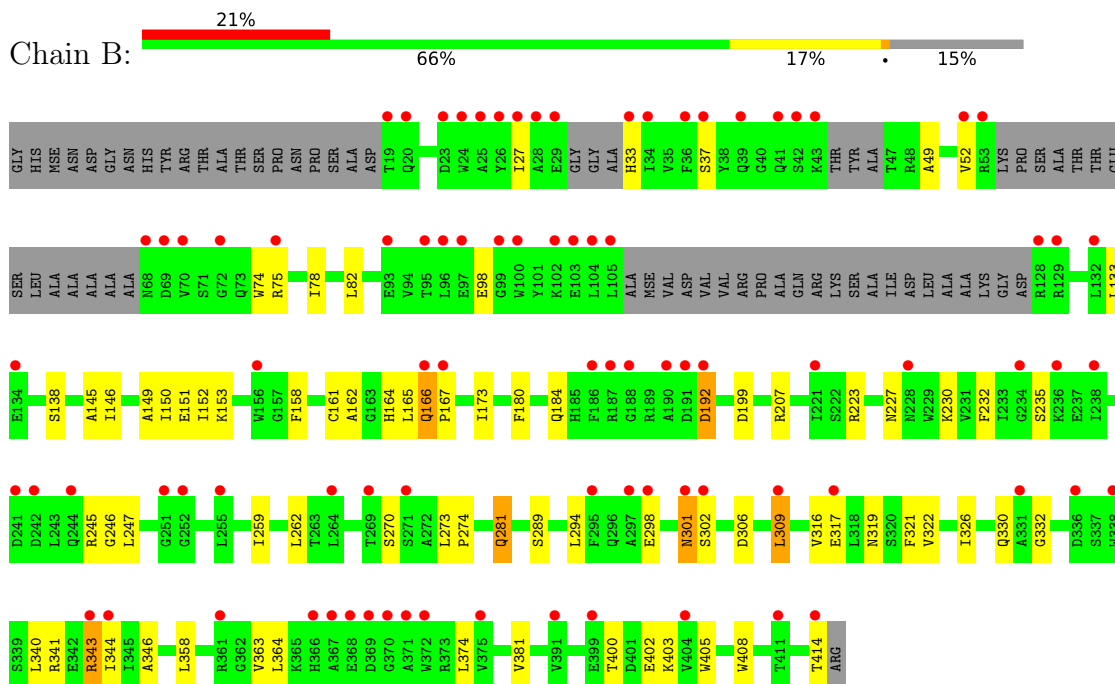
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inositol-pentakisphosphate 2-kinase



- Molecule 1: Inositol-pentakisphosphate 2-kinase



Chain C:

Amino Acid	Segment
ALA	Grey
ALA	Grey
ALA	Green
A66	Green
A67	Green
A68	Yellow
A69	Green
ASN	Green
ASN	Green
THR	Green
TYR	Green
ARG	Green
THR	Green
ALA	Green
THR	Green
SER	Green
P13	Green
M14	Green
P15	Yellow
S16	Yellow
A17	Green
D18	Green
T19	Yellow
Q20	Yellow
P21	Green
S22	Green
D23	Green
I27	Yellow
A28	Yellow
F29	Green
G30	Green
G31	Green
A32	Green
H33	Green
I34	Yellow
V35	Yellow
F36	Yellow
S37	Green
Y38	Green
G41	Green
S42	Green
K43	Green
T44	Yellow
V45	Green
A46	Green
T47	Green
L50	Grey
R51	Yellow
V52	Yellow
R53	Yellow
K54	Yellow
P55	Yellow
S56	Yellow
ALA	Grey
THR	Grey
THR	Grey
GLU	Grey
SER	Grey
LEU	Grey
ALA	Grey
ALA	Grey
LYS	Grey
GLY	Grey
D127	Green
R128	Green
G129	Green
G130	Green
V131	Green
D135	Yellow
S138	Yellow
D142	Green
D143	Green
K153	Green
P154	Green
K155	Green
P160	Green
L165	Yellow
Q166	Yellow
P167	Yellow
R179	Yellow
D192	Green
D196	Green
P197	Green
L198	Green
D199	Green
R207	Green
M208	Green
R209	Green
T210	Green
A211	Green
W219	Green
R223	Yellow
G224	Green
K225	Green
S226	Green
M227	Green
T233	Green
G234	Green
S235	Green
I238	Green
S239	Green
P240	Green
D241	Green
D242	Green
L243	Green
Q244	Green
L248	Green
G251	Green
T260	Green
Q261	Green
L262	Green
I266	Green

Chain D:

15% 75% 13% 10%

GLY HIS MSE ASN ASP GLY ASN HIS TYR ARG THR ALA THR SER P13 M14 P15 S16 A17 D18 W24 I27 A28 E29 G30 G31 A32 H33 I34 S37 Y38 K43 T44 Y45 V52 R53 R54 P55 S56 ALA THR THR GLU SER LEU ALA ALA ALA N68 D69 V70 S71 C72 R75 K81 R85 R92 E93 V94 E98 G99 W100 Y101 F102 F103 L104 L105 M107 V108 D109 V110 V111 ARG PRO ALA GLN ARG LYS SER ILE ASP LEU ALA ALA LYS GLY D127 R128 A129 G130 L133 A145 I146 I152 C161 A162 Q166 P167 P168 E169 L182 R187 G188 D191 P192 P193 P194 G214 M218 I233 I238 R245 G246 L247 L255 Q261 L262 L267 L286 A293 L294 F295 Q296 A297 E298 H299 P300 N301 S302 P303 I304 F305 D306 L309 E312 L318 F321 I326 S327 D328 R334 S337 L340 A346 L349 L358 V363 H366 A367 E368 D369 G370 S376 G377 K403 V404 W405 L409 R415

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.81Å 59.74Å 379.67Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	37.37 – 2.35 37.37 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.37-2.35) 98.8 (37.37-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.267 0.238 , 0.269	Depositor DCC
R_{free} test set	4401 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11782	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.36	0/2856	0.88	4/3873 (0.1%)
1	B	0.39	0/2731	0.90	10/3710 (0.3%)
1	C	0.40	0/3023	0.87	7/4099 (0.2%)
1	D	0.36	0/3005	0.89	5/4075 (0.1%)
All	All	0.38	0/11615	0.88	26/15757 (0.2%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLY	N-CA-C	-8.95	102.08	115.32
1	B	302	SER	CA-C-N	8.04	127.99	120.03
1	B	302	SER	C-N-CA	8.04	127.99	120.03
1	D	27	ILE	CB-CA-C	-7.38	105.43	111.71
1	A	166	GLN	CA-C-N	-7.09	113.08	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2802	0	2722	32	0
1	B	2676	0	2547	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2960	0	2929	50	0
1	D	2942	0	2906	35	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	10	0	0	1	0
3	A	75	0	0	3	0
3	B	37	0	0	1	0
3	C	149	0	0	5	0
3	D	96	0	0	4	0
All	All	11782	0	11104	156	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 7.

The worst 5 of 156 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:C:68:ASN:H	1:C:68:ASN:ND2	1.62	0.91
1:B:332:GLY:O	1:B:343:ARG:NH2	2.04	0.91
1:C:68:ASN:H	1:C:68:ASN:HD22	0.92	0.89
1:C:68:ASN:HD22	1:C:68:ASN:N	1.74	0.82
1:D:55:PRO:HD3	1:D:105:LEU:HD11	1.62	0.81

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	357/417 (86%)	346 (97%)	11 (3%)	0	100	100
1	B	344/417 (82%)	329 (96%)	12 (4%)	3 (1%)	14	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	373/417 (89%)	362 (97%)	10 (3%)	1 (0%)	36	43
1	D	371/417 (89%)	359 (97%)	8 (2%)	4 (1%)	11	11
All	All	1445/1668 (87%)	1396 (97%)	41 (3%)	8 (1%)	21	24

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	246	GLY
1	D	246	GLY
1	B	98	GLU
1	D	368	GLU
1	C	28	ALA

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	288/347 (83%)	276 (96%)	12 (4%)	26	35
1	B	270/347 (78%)	264 (98%)	6 (2%)	45	59
1	C	318/347 (92%)	308 (97%)	10 (3%)	35	47
1	D	314/347 (90%)	304 (97%)	10 (3%)	34	46
All	All	1190/1388 (86%)	1152 (97%)	38 (3%)	34	46

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	92	ARG
1	D	363	VAL
1	D	102	LYS
1	D	296	GLN
1	D	404	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	407	HIS
1	D	183	HIS
1	A	299	HIS
1	A	407	HIS
1	B	333	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	SO4	D	501	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	502	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	B	502	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.11	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
2	D	502	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	361/417 (86%)	1.40	89 (24%) 2 1	31, 54, 88, 102	0
1	B	349/417 (83%)	1.61	87 (24%) 2 1	42, 63, 92, 101	0
1	C	373/417 (89%)	0.78	57 (15%) 5 6	19, 36, 80, 96	0
1	D	371/417 (88%)	0.96	61 (16%) 4 5	20, 44, 78, 95	0
All	All	1454/1668 (87%)	1.18	294 (20%) 3 2	19, 52, 87, 102	0

The worst 5 of 294 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	LEU	8.9
1	A	108	VAL	8.0
1	B	367	ALA	7.8
1	C	66	ALA	7.6
1	D	108	VAL	6.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	503	5/5	0.85	0.13	67,74,86,95	0
2	SO4	A	502	5/5	0.86	0.10	79,98,116,119	0
2	SO4	A	501	5/5	0.86	0.16	62,67,82,86	0
2	SO4	B	502	5/5	0.90	0.13	60,79,84,85	0
2	SO4	B	501	5/5	0.94	0.08	54,59,68,70	0
2	SO4	C	502	5/5	0.95	0.10	47,56,66,69	0
2	SO4	D	501	5/5	0.95	0.11	52,55,63,64	0
2	SO4	D	502	5/5	0.95	0.14	41,52,56,75	0
2	SO4	C	501	5/5	0.98	0.06	40,43,50,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.