Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:47 pm BST

PDB ID	:	5XU6
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 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

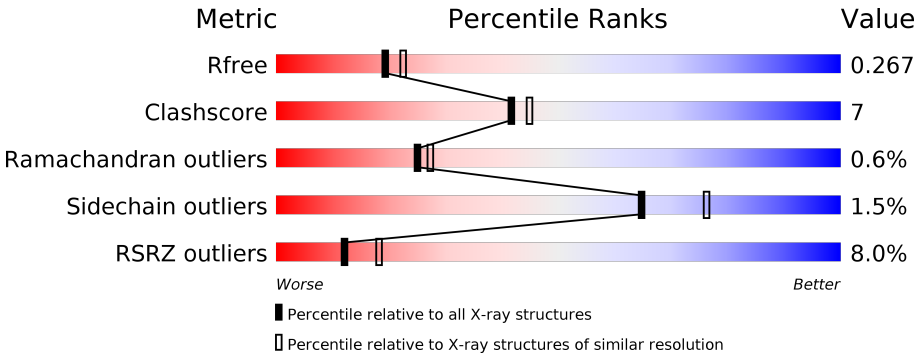
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 on 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 <=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	7% 76% 11% • 12%
1	B	417	10% 67% 17% • 15%
1	C	417	5% 73% 17% • 9%
1	D	417	7% 76% 15% 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.

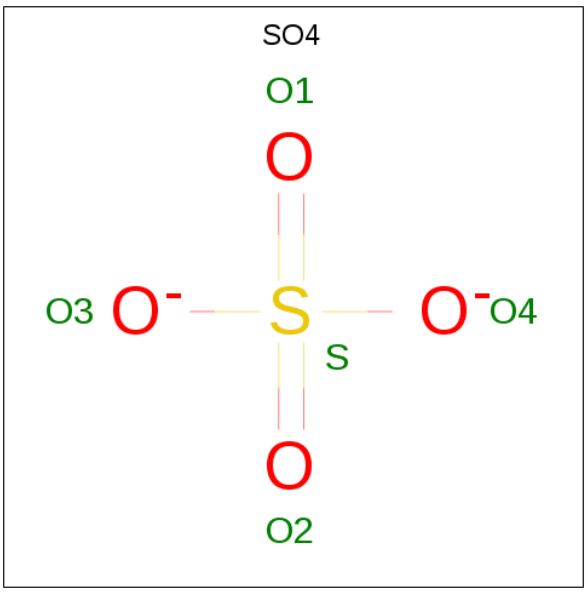
- Molecule 1 is a protein called Inositol-pentakisphosphate 2-kinase.

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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

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

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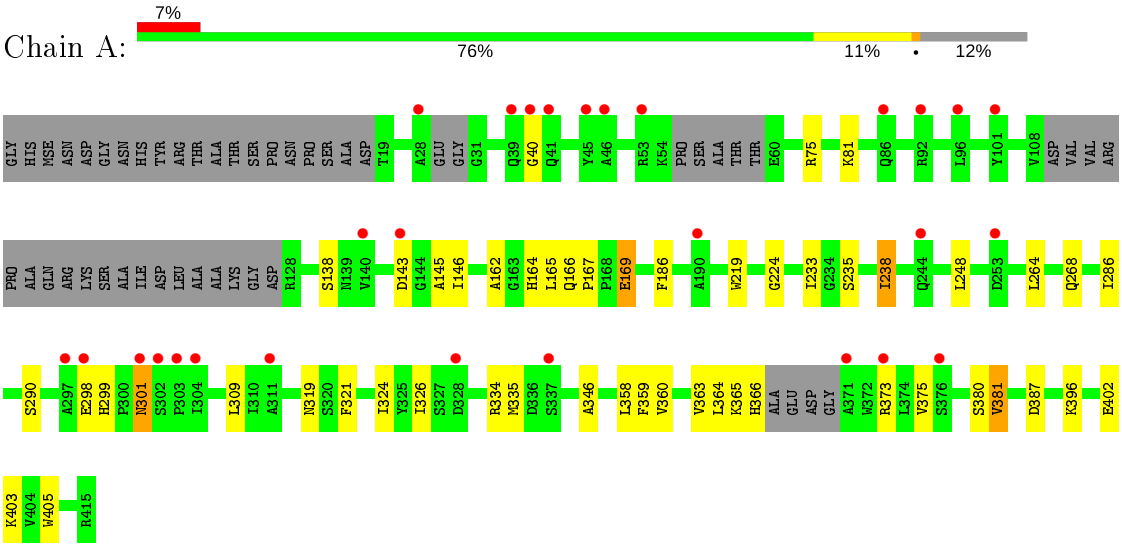
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	149	Total O 149 149	0	0
3	D	96	Total O 96 96	0	0

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 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.

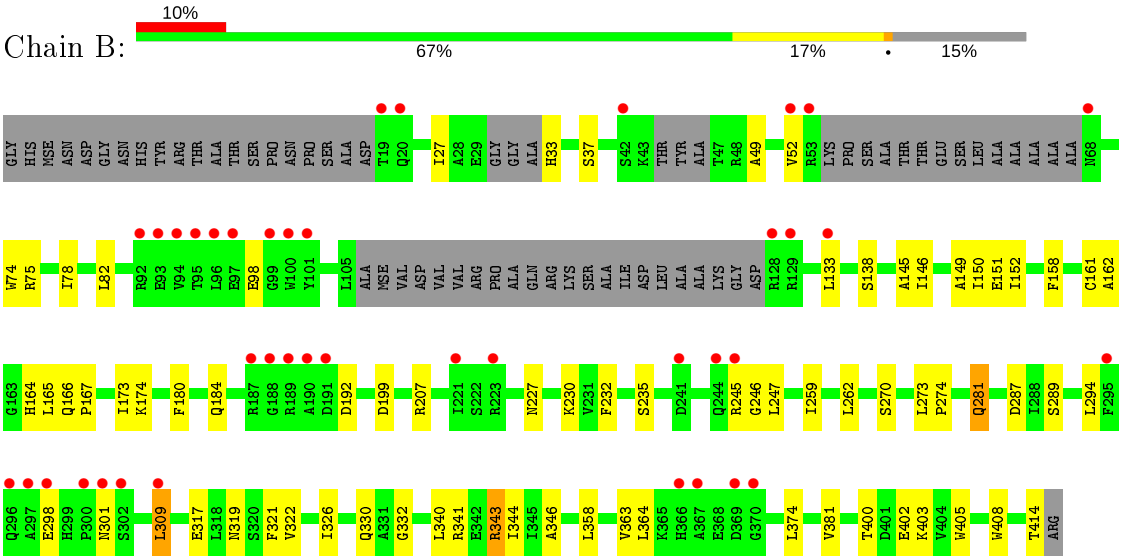
• Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain A:



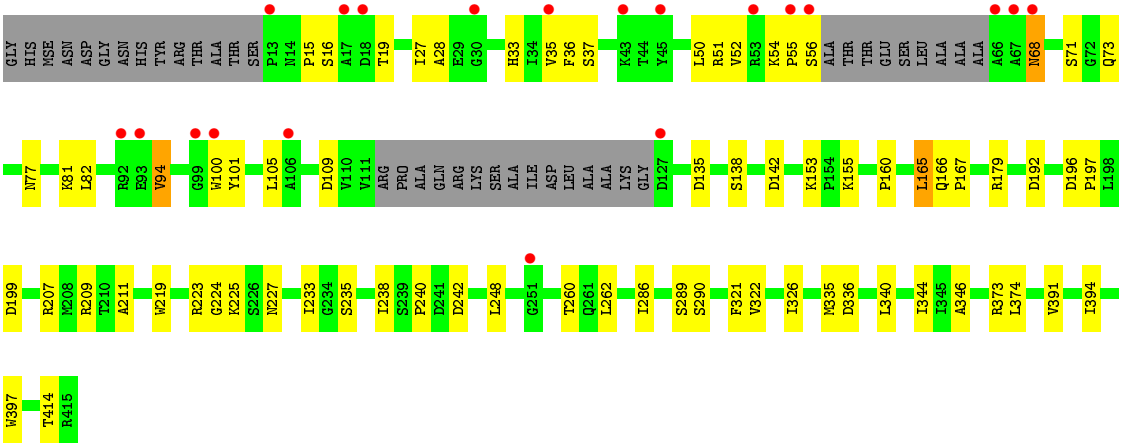
• Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain B:



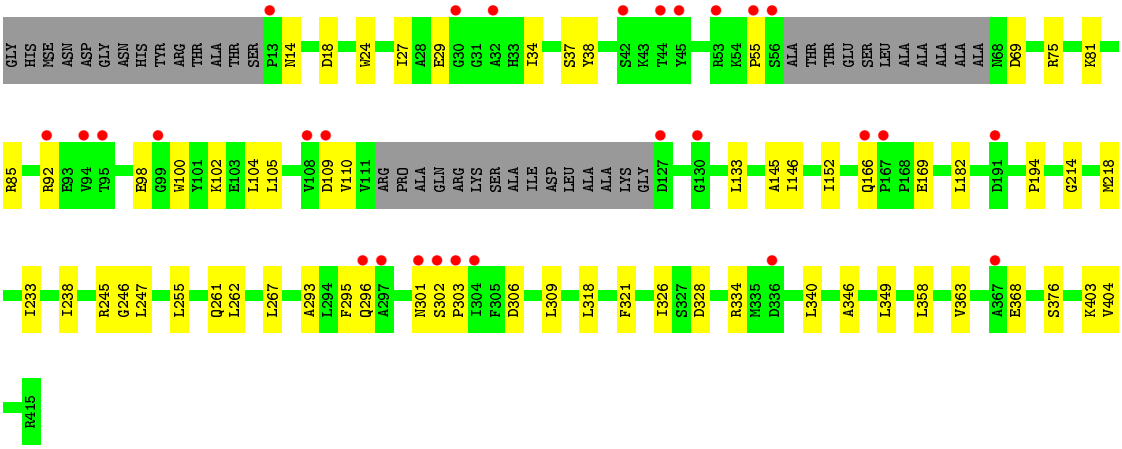
• Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain C:



- Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.267 0.237 , 0.267	Depositor DCC
R_{free} test set	4401 reflections (4.96%)	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 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.26	0/2856	0.52	0/3873
1	B	0.30	0/2731	0.51	0/3710
1	C	0.30	0/3023	0.53	0/4099
1	D	0.27	0/3005	0.53	0/4075
All	All	0.28	0/11615	0.52	0/15757

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2802	0	2722	32	0
1	B	2676	0	2547	44	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	157	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.

All (157) 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	0.97
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
1:B:27:ILE:HD11	1:B:37:SER:HB2	1.60	0.81
1:C:192:ASP:OD1	3:C:601:HOH:O	2.05	0.73
1:D:295:PHE:HA	1:D:340:LEU:HD11	1.70	0.73
1:D:182:LEU:HB3	1:D:404:VAL:HG13	1.71	0.73
1:A:138:SER:HA	1:A:235:SER:HB2	1.71	0.72
1:C:233:ILE:HD12	1:C:238:ILE:HG13	1.71	0.71
1:C:138:SER:HA	1:C:235:SER:HB2	1.72	0.71
1:C:68:ASN:ND2	1:C:68:ASN:N	2.38	0.69
1:D:245:ARG:O	1:D:247:LEU:N	2.27	0.68
1:C:73:GLN:OE1	1:C:77:ASN:ND2	2.27	0.67
1:A:166:GLN:HB3	1:A:167:PRO:HD3	1.77	0.66
1:D:233:ILE:HD12	1:D:238:ILE:HG13	1.76	0.66
1:D:81:LYS:HB3	1:D:326:ILE:HD11	1.78	0.66
1:B:301:ASN:OD1	1:B:301:ASN:N	2.28	0.65
1:D:152:ILE:HG23	1:D:358:LEU:HB2	1.77	0.65
1:C:290:SER:OG	1:D:109:ASP:OD2	2.13	0.65
1:D:29:GLU:HG3	1:D:34:ILE:HG12	1.77	0.64
1:B:270:SER:HB2	1:B:381:VAL:HG11	1.79	0.64
1:B:152:ILE:HG23	1:B:358:LEU:HB2	1.80	0.63
1:A:40:GLY:HA3	1:B:162:ALA:HB2	1.80	0.63
1:C:153:LYS:NZ	1:C:227:ASN:HB3	2.15	0.62
1:B:33:HIS:N	1:B:52:VAL:O	2.33	0.62
1:C:81:LYS:HB3	1:C:326:ILE:HD11	1.82	0.61
1:D:328:ASP:OD2	1:D:334:ARG:NH2	2.34	0.61
1:D:85:ARG:NH2	3:D:605:HOH:O	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:HA	1:C:71:SER:OG	2.01	0.60
1:C:27:ILE:HD11	1:C:37:SER:HB2	1.83	0.60
1:C:35:VAL:HG22	1:C:51:ARG:HG3	1.84	0.59
1:B:146:ILE:HD12	1:B:364:LEU:HD23	1.85	0.59
1:C:54:LYS:HD2	1:C:55:PRO:HD2	1.85	0.58
1:A:81:LYS:NZ	1:A:319:ASN:OD1	2.34	0.58
1:C:286:ILE:HD13	1:C:335:MSE:HE1	1.85	0.57
1:D:145:ALA:HB1	1:D:363:VAL:HG13	1.87	0.57
1:C:15:PRO:O	1:C:19:THR:OG1	2.15	0.57
1:B:158:PHE:CG	1:B:281:GLN:HG3	2.40	0.56
1:D:245:ARG:O	1:D:247:LEU:HG	2.05	0.56
1:D:267:LEU:O	3:D:602:HOH:O	2.18	0.55
1:A:75:ARG:NH1	1:A:387:ASP:OD1	2.39	0.55
1:A:169:GLU:O	3:A:601:HOH:O	2.18	0.55
1:B:151:GLU:HB3	1:B:230:LYS:HB2	1.89	0.55
1:A:396:LYS:NZ	2:A:501:SO4:O1	2.38	0.55
1:A:402:GLU:HA	1:A:405:TRP:CD1	2.42	0.55
1:B:166:GLN:HB2	1:B:289:SER:HB3	1.90	0.54
1:B:330:GLN:NE2	3:B:601:HOH:O	2.27	0.54
1:C:166:GLN:HB2	1:C:167:PRO:HD3	1.90	0.54
1:B:245:ARG:O	1:B:247:LEU:HG	2.08	0.54
1:C:135:ASP:OD2	3:C:602:HOH:O	2.18	0.53
1:D:98:GLU:OE2	3:D:601:HOH:O	2.18	0.53
1:B:402:GLU:HA	1:B:405:TRP:CD1	2.43	0.53
1:A:233:ILE:HG13	1:A:238:ILE:HD12	1.89	0.53
1:C:262:LEU:HD13	1:C:374:LEU:HG	1.91	0.53
1:A:366:HIS:O	3:A:602:HOH:O	2.19	0.53
1:B:270:SER:CB	1:B:381:VAL:HG11	2.39	0.53
1:B:294:LEU:O	1:B:298:GLU:HG3	2.09	0.52
1:B:49:ALA:HB3	1:B:133:LEU:HB2	1.92	0.52
1:B:161:CYS:SG	1:B:164:HIS:ND1	2.82	0.52
1:B:317:GLU:OE2	1:B:341:ARG:NE	2.36	0.52
1:B:173:ILE:HD11	1:B:414:THR:HA	1.92	0.51
1:B:227:ASN:OD1	1:B:230:LYS:HE3	2.10	0.51
1:C:82:LEU:HD21	1:C:322:VAL:HG13	1.92	0.51
1:D:306:ASP:HB3	1:D:309:LEU:HD13	1.93	0.50
1:C:52:VAL:HG11	1:C:101:TYR:HE1	1.76	0.50
1:A:359:PHE:O	1:A:381:VAL:HA	2.12	0.50
1:D:75:ARG:NH2	2:D:502:SO4:O2	2.42	0.50
1:A:301:ASN:ND2	3:A:607:HOH:O	2.32	0.50
1:C:223:ARG:HA	1:C:240:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLN:HG3	1:C:289:SER:O	2.12	0.49
1:A:365:LYS:HD2	1:A:375:VAL:HG21	1.93	0.49
1:B:400:THR:HA	1:B:403:LYS:HE3	1.94	0.49
1:A:360:VAL:HA	1:A:380:SER:O	2.11	0.49
1:B:146:ILE:HB	1:B:364:LEU:HB3	1.94	0.49
1:D:100:TRP:HZ3	1:D:104:LEU:HD22	1.78	0.49
1:D:27:ILE:HD11	1:D:37:SER:HB2	1.95	0.49
1:C:209:ARG:NH1	1:C:260:THR:HG21	2.28	0.48
1:B:262:LEU:HD13	1:B:374:LEU:HG	1.95	0.48
1:A:186:PHE:CZ	1:A:403:LYS:HD3	2.47	0.48
1:D:100:TRP:CZ3	1:D:104:LEU:HD22	2.48	0.48
1:B:199:ASP:HA	1:B:207:ARG:HE	1.79	0.48
1:C:414:THR:HG23	1:D:146:ILE:HG12	1.96	0.48
1:B:321:PHE:CZ	1:B:346:ALA:HB2	2.48	0.48
1:B:162:ALA:HA	1:B:165:LEU:HD12	1.96	0.48
1:B:82:LEU:HD21	1:B:322:VAL:HG13	1.96	0.48
1:B:180:PHE:O	1:B:184:GLN:HG2	2.14	0.47
1:C:142:ASP:N	1:C:142:ASP:OD1	2.46	0.47
1:B:173:ILE:HD12	1:B:408:TRP:CD1	2.49	0.47
1:A:219:TRP:CD1	1:A:224:GLY:HA2	2.50	0.47
1:C:179:ARG:NH2	3:C:609:HOH:O	2.35	0.47
1:C:166:GLN:OE1	1:D:110:VAL:HA	2.14	0.47
1:A:164:HIS:CD2	1:A:286:ILE:HG22	2.50	0.47
1:C:233:ILE:HG21	1:C:248:LEU:HD11	1.97	0.47
1:D:262:LEU:CD1	1:D:376:SER:HB2	2.46	0.46
1:D:318:LEU:HD11	1:D:349:LEU:HD21	1.98	0.46
1:B:138:SER:HA	1:B:235:SER:OG	2.15	0.46
1:B:174:LYS:NZ	1:B:287:ASP:OD1	2.40	0.46
1:B:273:LEU:HB2	1:B:274:PRO:HD3	1.99	0.45
1:A:298:GLU:O	1:A:299:HIS:HD2	1.99	0.45
1:B:74:TRP:CD1	1:B:75:ARG:HG2	2.51	0.45
1:A:321:PHE:CZ	1:A:346:ALA:HB2	2.52	0.45
1:D:14:ASN:O	1:D:18:ASP:N	2.41	0.45
1:C:160:PRO:HB2	1:C:165:LEU:HD11	1.99	0.44
1:A:233:ILE:HG21	1:A:248:LEU:HD11	2.00	0.44
1:A:264:LEU:O	1:A:268:GLN:HG3	2.16	0.44
1:B:402:GLU:HA	1:B:405:TRP:NE1	2.33	0.44
1:A:162:ALA:HA	1:A:165:LEU:HD12	1.99	0.44
1:B:150:ILE:HD11	1:B:259:ILE:HD13	2.00	0.44
1:A:286:ILE:O	1:A:290:SER:HB2	2.18	0.44
1:C:321:PHE:CZ	1:C:346:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:LEU:O	1:B:344:ILE:HG13	2.18	0.43
1:D:403:LYS:HE3	1:D:403:LYS:HB2	1.72	0.43
1:C:336:ASP:OD1	1:C:336:ASP:N	2.51	0.43
1:B:166:GLN:HB2	1:B:167:PRO:HD3	2.01	0.43
1:D:233:ILE:HD13	1:D:255:LEU:HD21	2.00	0.43
1:B:145:ALA:HB1	1:B:363:VAL:HG13	1.99	0.43
1:B:326:ILE:HA	1:B:326:ILE:HD13	1.86	0.43
1:C:15:PRO:HG2	1:C:94:VAL:HG21	2.01	0.43
1:C:394:ILE:HA	1:C:397:TRP:CE3	2.54	0.43
1:D:105:LEU:HD23	1:D:105:LEU:O	2.19	0.43
1:C:36:PHE:N	1:C:50:LEU:O	2.51	0.42
1:C:196:ASP:HA	1:C:197:PRO:HD2	1.94	0.42
1:A:143:ASP:HB3	1:A:145:ALA:H	1.84	0.42
1:A:299:HIS:ND1	1:A:309:LEU:HD13	2.33	0.42
1:D:321:PHE:CZ	1:D:346:ALA:HB2	2.54	0.42
1:A:81:LYS:HB3	1:A:326:ILE:HD11	2.01	0.42
1:A:358:LEU:HD12	1:A:358:LEU:HA	1.88	0.42
1:A:146:ILE:HD12	1:A:364:LEU:HD23	2.00	0.42
1:C:199:ASP:HB3	1:C:207:ARG:O	2.20	0.42
1:D:24:TRP:CZ3	1:D:38:TYR:HB2	2.55	0.41
1:A:334:ARG:O	1:A:335:MSE:HE2	2.20	0.41
1:C:225:LYS:HE2	1:C:225:LYS:HB2	1.89	0.41
1:C:56:SER:HA	1:C:105:LEU:HD23	2.02	0.41
1:B:245:ARG:O	1:B:247:LEU:N	2.54	0.41
1:C:373:ARG:NH2	3:C:623:HOH:O	2.53	0.41
1:C:16:SER:HA	1:C:100:TRP:CD1	2.55	0.41
1:A:169:GLU:HG3	1:A:169:GLU:H	1.60	0.41
1:B:309:LEU:HD23	1:B:309:LEU:O	2.21	0.41
1:D:302:SER:HB3	1:D:303:PRO:HD2	2.02	0.41
1:D:166:GLN:OE1	1:D:293:ALA:HB2	2.20	0.41
1:A:146:ILE:HB	1:A:364:LEU:HB3	2.02	0.41
1:D:261:GLN:NE2	3:D:610:HOH:O	2.43	0.41
1:B:149:ALA:HB3	1:B:232:PHE:HB2	2.03	0.41
1:C:219:TRP:CD1	1:C:224:GLY:HA2	2.56	0.41
1:B:78:ILE:HD12	1:B:319:ASN:HB2	2.02	0.40
1:C:153:LYS:HZ3	1:C:227:ASN:HB3	1.85	0.40
1:C:238:ILE:HG23	1:C:242:ASP:HB2	2.02	0.40
1:D:194:PRO:HB2	1:D:214:GLY:HA2	2.03	0.40
1:D:194:PRO:HG2	1:D:218:MSE:HG3	2.03	0.40
1:C:153:LYS:HB3	1:C:155:LYS:HE3	2.04	0.40
1:A:145:ALA:HB1	1:A:363:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:HIS:HB3	1:C:52:VAL:O	2.20	0.40
1:C:344:ILE:HG22	1:C:391:VAL:CG2	2.52	0.40
1:C:211:ALA:HA	3:C:662:HOH:O	2.22	0.40
1:C:340:LEU:O	1:C:344:ILE:HG13	2.21	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	357/417 (86%)	346 (97%)	11 (3%)	0	100	100
1	B	344/417 (82%)	329 (96%)	12 (4%)	3 (1%)	17	17
1	C	373/417 (89%)	362 (97%)	10 (3%)	1 (0%)	41	47
1	D	371/417 (89%)	359 (97%)	8 (2%)	4 (1%)	14	13
All	All	1445/1668 (87%)	1396 (97%)	41 (3%)	8 (1%)	25	27

All (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
1	D	301	ASN
1	D	69	ASP
1	B	192	ASP

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	288/347 (83%)	282 (98%)	6 (2%)	53	65
1	B	270/347 (78%)	267 (99%)	3 (1%)	73	84
1	C	318/347 (92%)	314 (99%)	4 (1%)	69	80
1	D	314/347 (90%)	309 (98%)	5 (2%)	62	75
All	All	1190/1388 (86%)	1172 (98%)	18 (2%)	65	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	GLU
1	A	238	ILE
1	A	301	ASN
1	A	324	ILE
1	A	373	ARG
1	A	381	VAL
1	B	281	GLN
1	B	309	LEU
1	B	343	ARG
1	C	68	ASN
1	C	94	VAL
1	C	109	ASP
1	C	165	LEU
1	D	92	ARG
1	D	102	LYS
1	D	133	LEU
1	D	169	GLU
1	D	296	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS

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Mol	Chain	Res	Type
1	C	68	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	C	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	501	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.06	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

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^{th} 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%)	0.58	28 (7%) 13 19	31, 54, 88, 102	0
1	B	349/417 (83%)	0.68	40 (11%) 4 7	42, 63, 92, 101	0
1	C	373/417 (89%)	0.44	20 (5%) 25 37	19, 36, 80, 96	0
1	D	371/417 (88%)	0.48	28 (7%) 14 21	20, 44, 78, 95	0
All	All	1454/1668 (87%)	0.54	116 (7%) 12 18	19, 52, 87, 102	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	LEU	6.7
1	B	68	ASN	6.4
1	C	55	PRO	6.3
1	C	43	LYS	6.2
1	B	95	THR	5.7
1	B	100	TRP	5.5
1	A	302	SER	5.4
1	B	302	SER	5.1
1	B	97	GLU	5.0
1	B	92	ARG	4.8
1	C	106	ALA	4.7
1	C	13	PRO	4.7
1	A	304	ILE	4.5
1	C	66	ALA	4.5
1	A	46	ALA	4.5
1	A	40	GLY	4.4
1	B	99	GLY	4.4
1	B	300	PRO	4.3
1	B	367	ALA	4.2
1	A	53	ARG	4.1
1	B	93	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	244	GLN	4.0
1	D	56	SER	4.0
1	A	39	GLN	3.9
1	D	367	ALA	3.9
1	D	109	ASP	3.8
1	A	373	ARG	3.8
1	B	190	ALA	3.7
1	D	55	PRO	3.7
1	A	140	VAL	3.6
1	D	127	ASP	3.6
1	C	92	ARG	3.5
1	D	304	ILE	3.5
1	A	303	PRO	3.5
1	A	311	ALA	3.5
1	A	371	ALA	3.4
1	B	94	VAL	3.4
1	D	191	ASP	3.3
1	B	19	THR	3.3
1	A	301	ASN	3.3
1	D	130	GLY	3.3
1	B	370	GLY	3.2
1	B	297	ALA	3.2
1	A	190	ALA	3.1
1	C	68	ASN	3.1
1	A	86	GLN	3.1
1	D	53	ARG	3.0
1	D	296	GLN	3.0
1	D	302	SER	3.0
1	B	223	ARG	3.0
1	B	101	TYR	3.0
1	C	17	ALA	2.9
1	D	92	ARG	2.9
1	D	301	ASN	2.9
1	B	241	ASP	2.9
1	A	297	ALA	2.8
1	A	92	ARG	2.8
1	B	369	ASP	2.8
1	B	129	ARG	2.8
1	D	303	PRO	2.7
1	D	32	ALA	2.7
1	B	191	ASP	2.7
1	B	187	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	296	GLN	2.6
1	A	376	SER	2.6
1	B	42	SER	2.6
1	D	95	THR	2.6
1	C	93	GLU	2.6
1	C	251	GLY	2.5
1	B	309	LEU	2.5
1	B	245	ARG	2.5
1	D	297	ALA	2.5
1	D	42	SER	2.5
1	A	28	ALA	2.4
1	B	133	LEU	2.4
1	B	295	PHE	2.4
1	B	128	ARG	2.4
1	D	45	TYR	2.4
1	C	45	TYR	2.4
1	C	100	TRP	2.4
1	B	20	GLN	2.4
1	B	188	GLY	2.4
1	A	337	SER	2.4
1	B	366	HIS	2.3
1	A	143	ASP	2.3
1	D	167	PRO	2.3
1	C	53	ARG	2.2
1	D	336	ASP	2.2
1	D	13	PRO	2.2
1	B	221	ILE	2.2
1	A	328	ASP	2.2
1	C	18	ASP	2.2
1	C	35	VAL	2.2
1	D	108	VAL	2.2
1	B	301	ASN	2.2
1	A	298	GLU	2.2
1	B	53	ARG	2.2
1	B	298	GLU	2.2
1	A	41	GLN	2.2
1	A	45	TYR	2.2
1	C	99	GLY	2.2
1	D	166	GLN	2.2
1	B	52	VAL	2.1
1	C	127	ASP	2.1
1	C	30	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	189	ARG	2.1
1	A	101	TYR	2.1
1	A	253	ASP	2.1
1	D	94	VAL	2.1
1	C	56	SER	2.1
1	A	96	LEU	2.1
1	D	30	GLY	2.1
1	D	44	THR	2.0
1	D	99	GLY	2.0
1	A	244	GLN	2.0
1	C	67	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
2	SO4	C	503	5/5	0.89	0.15	67,74,86,95	0
2	SO4	A	502	5/5	0.93	0.17	79,98,116,119	0
2	SO4	B	502	5/5	0.96	0.12	60,79,84,85	0
2	SO4	C	502	5/5	0.96	0.11	47,56,66,69	0
2	SO4	A	501	5/5	0.97	0.12	62,67,82,86	0
2	SO4	B	501	5/5	0.97	0.07	54,59,68,70	0
2	SO4	D	501	5/5	0.97	0.11	52,55,63,64	0
2	SO4	D	502	5/5	0.98	0.09	41,52,56,75	0
2	SO4	C	501	5/5	0.99	0.10	40,43,50,58	0

6.5 Other polymers (i)

There are no such residues in this entry.