



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:48 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 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 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

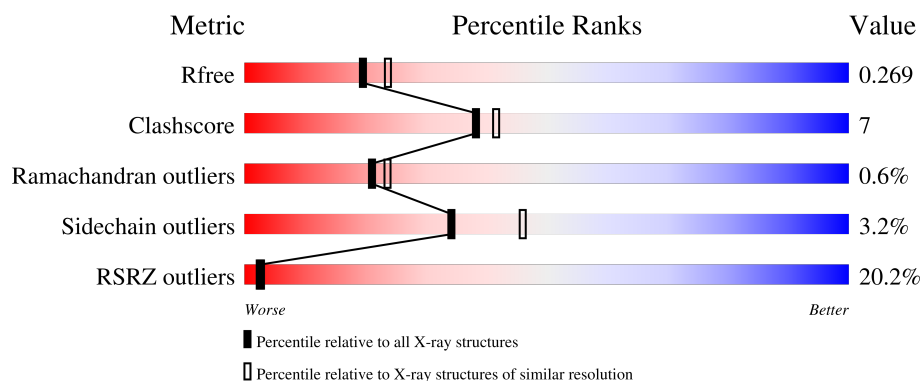
1 Overall quality at a glance

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.

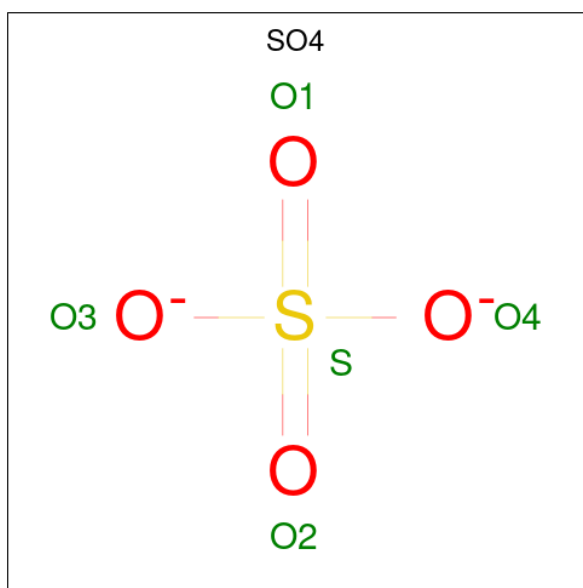
- Molecule 1 is a protein called Inositol-pentakisphosphate 2-kinase.

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

Chain C:

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 ⓘ

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	0.36	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.

All (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
1	A	166	GLN	C-N-CA	-7.09	113.08	120.38
1	D	166	GLN	CA-C-N	-6.89	113.29	120.38
1	D	166	GLN	C-N-CA	-6.89	113.29	120.38
1	C	166	GLN	CA-C-N	-6.87	113.30	120.38
1	C	166	GLN	C-N-CA	-6.87	113.30	120.38
1	C	27	ILE	CB-CA-C	-6.84	103.42	110.88
1	C	31	GLY	N-CA-C	-6.69	104.41	113.37
1	B	166	GLN	CA-C-N	-6.52	113.67	120.38
1	B	166	GLN	C-N-CA	-6.52	113.67	120.38
1	B	192	ASP	CA-C-N	-6.16	114.03	120.38
1	B	192	ASP	C-N-CA	-6.16	114.03	120.38
1	B	153	LYS	CA-C-N	5.93	125.48	119.19
1	B	153	LYS	C-N-CA	5.93	125.48	119.19
1	D	14	ASN	CA-C-N	5.25	124.88	119.05
1	D	14	ASN	C-N-CA	5.25	124.88	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	THR	N-CA-C	-5.20	103.82	110.53
1	C	54	LYS	CA-C-N	5.14	127.48	120.79
1	C	54	LYS	C-N-CA	5.14	127.48	120.79
1	B	306	ASP	CA-C-N	5.10	124.89	119.28
1	B	306	ASP	C-N-CA	5.10	124.89	119.28
1	C	73	GLN	CA-CB-CG	-5.07	103.96	114.10

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	43	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
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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:301:ASN:OD1	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
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:15:PRO:O	1:C:19:THR:OG1	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:27:ILE:HD11	1:D:37:SER:HB2	1.95	0.49
1:D:100:TRP:HZ3	1:D:104:LEU:HD22	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:340:LEU:O	1:B:344:ILE:HG13	2.18	0.43
1:D:403:LYS:HB2	1:D:403:LYS:HE3	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:HD13	1:B:326:ILE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:SER:HA	1:C:105:LEU:HD23	2.02	0.41
1:C:225:LYS:HE2	1:C:225:LYS:HB2	1.89	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:H	1:A:169:GLU:HG3	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:C:153:LYS:HZ2	1:C:227:ASN:HB3	1.83	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: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
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 ⓘ

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

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 ⓘ

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

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	95	THR
1	A	98	GLU
1	A	169	GLU
1	A	231	VAL
1	A	238	ILE
1	A	261	GLN
1	A	301	ASN
1	A	324	ILE
1	A	358	LEU
1	A	373	ARG
1	A	381	VAL
1	B	223	ARG
1	B	281	GLN
1	B	301	ASN
1	B	309	LEU
1	B	316	VAL
1	B	343	ARG
1	C	35	VAL
1	C	44	THR
1	C	68	ASN
1	C	94	VAL
1	C	102	LYS
1	C	108	VAL
1	C	109	ASP
1	C	165	LEU
1	C	223	ARG
1	C	244	GLN
1	D	92	ARG
1	D	102	LYS
1	D	133	LEU
1	D	169	GLU
1	D	296	GLN
1	D	301	ASN
1	D	312	GLU
1	D	363	VAL
1	D	368	GLU
1	D	404	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN

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Mol	Chain	Res	Type
1	A	164	HIS
1	A	228	ASN
1	A	299	HIS
1	A	407	HIS
1	B	333	GLN
1	C	68	ASN
1	C	407	HIS
1	D	183	HIS

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
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

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	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

All (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
1	C	32	ALA	6.4
1	A	40	GLY	6.0
1	D	367	ALA	5.7
1	C	106	ALA	5.7
1	D	13	PRO	5.7
1	A	38	TYR	5.4
1	A	46	ALA	5.4
1	D	127	ASP	5.4
1	B	19	THR	5.4
1	C	13	PRO	5.2
1	A	101	TYR	5.2
1	D	109	ASP	5.1
1	B	43	LYS	5.0
1	A	39	GLN	4.9
1	A	19	THR	4.9
1	A	28	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	371	ALA	4.7
1	C	143	ASP	4.7
1	A	297	ALA	4.7
1	D	111	VAL	4.7
1	B	252	GLY	4.6
1	B	190	ALA	4.6
1	B	68	ASN	4.6
1	A	96	LEU	4.5
1	D	167	PRO	4.4
1	B	33	HIS	4.3
1	C	35	VAL	4.3
1	D	69	ASP	4.3
1	C	108	VAL	4.2
1	A	190	ALA	4.2
1	A	99	GLY	4.2
1	A	41	GLN	4.2
1	A	45	TYR	4.2
1	C	44	THR	4.1
1	A	140	VAL	4.1
1	D	31	GLY	4.1
1	A	27	ILE	4.1
1	A	238	ILE	4.1
1	A	128	ARG	4.0
1	B	97	GLU	4.0
1	C	69	ASP	4.0
1	C	55	PRO	3.9
1	B	191	ASP	3.9
1	D	191	ASP	3.9
1	A	167	PRO	3.9
1	D	106	ALA	3.9
1	B	69	ASP	3.8
1	A	44	THR	3.8
1	B	27	ILE	3.8
1	A	246	GLY	3.8
1	D	327	SER	3.8
1	A	106	ALA	3.8
1	D	301	ASN	3.8
1	C	56	SER	3.8
1	C	251	GLY	3.8
1	C	67	ALA	3.7
1	B	24	TRP	3.7
1	B	104	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	42	SER	3.7
1	C	30	GLY	3.6
1	C	127	ASP	3.6
1	C	93	GLU	3.6
1	B	20	GLN	3.5
1	C	27	ILE	3.5
1	B	95	THR	3.5
1	A	161	CYS	3.5
1	A	91	SER	3.5
1	A	130	GLY	3.5
1	C	68	ASN	3.5
1	A	293	ALA	3.4
1	B	99	GLY	3.4
1	D	102	LYS	3.4
1	A	35	VAL	3.4
1	D	110	VAL	3.4
1	A	103	GLU	3.4
1	A	304	ILE	3.4
1	B	41	GLN	3.4
1	A	376	SER	3.4
1	A	102	LYS	3.4
1	D	303	PRO	3.3
1	D	71	SER	3.3
1	B	269	THR	3.3
1	D	56	SER	3.3
1	C	19	THR	3.3
1	C	166	GLN	3.3
1	A	311	ALA	3.3
1	B	368	GLU	3.3
1	B	100	TRP	3.3
1	A	168	PRO	3.2
1	C	42	SER	3.2
1	A	241	ASP	3.2
1	D	304	ILE	3.2
1	D	296	GLN	3.2
1	D	297	ALA	3.2
1	D	130	GLY	3.2
1	C	43	LYS	3.2
1	B	370	GLY	3.2
1	C	52	VAL	3.2
1	D	33	HIS	3.2
1	B	242	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	302	SER	3.1
1	B	102	LYS	3.1
1	A	137	THR	3.1
1	D	68	ASN	3.1
1	D	32	ALA	3.1
1	D	295	PHE	3.0
1	B	96	LEU	3.0
1	C	98	GLU	3.0
1	B	26	TYR	3.0
1	A	300	PRO	3.0
1	B	371	ALA	3.0
1	B	369	ASP	3.0
1	B	372	TRP	3.0
1	A	143	ASP	3.0
1	B	188	GLY	3.0
1	D	166	GLN	2.9
1	D	337	SER	2.9
1	B	297	ALA	2.9
1	B	39	GLN	2.9
1	A	301	ASN	2.9
1	B	234	GLY	2.9
1	D	72	GLY	2.9
1	A	331	ALA	2.9
1	A	295	PHE	2.9
1	D	93	GLU	2.9
1	B	34	ILE	2.9
1	B	375	VAL	2.8
1	A	324	ILE	2.8
1	B	72	GLY	2.8
1	B	70	VAL	2.8
1	A	95	THR	2.8
1	B	343	ARG	2.8
1	C	53	ARG	2.8
1	B	366	HIS	2.8
1	A	129	ARG	2.8
1	C	129	ARG	2.8
1	D	53	ARG	2.8
1	A	366	HIS	2.8
1	C	34	ILE	2.8
1	D	30	GLY	2.8
1	A	136	LEU	2.8
1	B	28	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	17	ALA	2.8
1	A	52	VAL	2.8
1	A	86	GLN	2.7
1	C	23	ASP	2.7
1	A	303	PRO	2.7
1	B	53	ARG	2.7
1	A	296	GLN	2.7
1	A	31	GLY	2.7
1	A	245	ARG	2.7
1	D	92	ARG	2.7
1	A	131	VAL	2.7
1	D	94	VAL	2.7
1	A	234	GLY	2.7
1	B	238	ILE	2.7
1	A	337	SER	2.7
1	B	302	SER	2.7
1	D	55	PRO	2.7
1	B	298	GLU	2.7
1	C	97	GLU	2.7
1	A	163	GLY	2.7
1	D	161	CYS	2.7
1	A	105	LEU	2.7
1	A	328	ASP	2.6
1	B	192	ASP	2.6
1	B	301	ASN	2.6
1	B	251	GLY	2.6
1	D	187	ARG	2.6
1	D	286	ILE	2.6
1	A	254	ASP	2.6
1	A	299	HIS	2.6
1	D	133	LEU	2.6
1	A	97	GLU	2.6
1	B	128	ARG	2.6
1	C	336	ASP	2.6
1	D	192	ASP	2.6
1	D	188	GLY	2.6
1	A	235	SER	2.6
1	B	309	LEU	2.6
1	A	139	ASN	2.6
1	B	331	ALA	2.5
1	A	253	ASP	2.5
1	C	111	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	336	ASP	2.5
1	C	192	ASP	2.5
1	D	18	ASP	2.5
1	A	42	SER	2.5
1	D	104	LEU	2.5
1	C	54	LYS	2.5
1	D	43	LYS	2.5
1	A	142	ASP	2.5
1	C	244	GLN	2.5
1	A	98	GLU	2.4
1	B	75	ARG	2.4
1	B	391	VAL	2.4
1	A	104	LEU	2.4
1	C	142	ASP	2.4
1	C	46	ALA	2.4
1	C	368	GLU	2.4
1	B	186	PHE	2.4
1	C	94	VAL	2.4
1	A	92	ARG	2.4
1	C	128	ARG	2.4
1	B	25	ALA	2.4
1	C	105	LEU	2.4
1	D	405	TRP	2.4
1	A	33	HIS	2.4
1	A	20	GLN	2.4
1	A	85	ARG	2.4
1	D	129	ARG	2.4
1	B	93	GLU	2.4
1	D	369	ASP	2.4
1	B	167	PRO	2.4
1	C	95	THR	2.4
1	D	409	LEU	2.4
1	A	298	GLU	2.4
1	B	23	ASP	2.3
1	C	22	SER	2.3
1	B	134	GLU	2.3
1	B	166	GLN	2.3
1	C	41	GLN	2.3
1	B	228	ASN	2.3
1	C	38	TYR	2.3
1	A	32	ALA	2.3
1	A	145	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	411	THR	2.3
1	A	166	GLN	2.3
1	B	404	VAL	2.3
1	B	264	LEU	2.3
1	C	241	ASP	2.3
1	D	45	TYR	2.3
1	A	269	THR	2.3
1	C	235	SER	2.3
1	D	16	SER	2.3
1	B	132	LEU	2.3
1	C	14	ASN	2.3
1	B	187	ARG	2.3
1	B	129	ARG	2.2
1	C	92	ARG	2.2
1	C	47	THR	2.2
1	A	100	TRP	2.2
1	C	91	SER	2.2
1	B	103	GLU	2.2
1	B	244	GLN	2.2
1	C	28	ALA	2.2
1	A	61	SER	2.2
1	D	302	SER	2.2
1	A	24	TRP	2.2
1	B	221	ILE	2.2
1	C	131	VAL	2.2
1	B	295	PHE	2.2
1	D	370	GLY	2.2
1	C	101	TYR	2.2
1	D	105	LEU	2.2
1	D	52	VAL	2.2
1	B	29	GLU	2.2
1	D	366	HIS	2.2
1	A	90	THR	2.2
1	D	162	ALA	2.2
1	A	48	ARG	2.1
1	B	255	LEU	2.1
1	C	20	GLN	2.1
1	A	377	GLY	2.1
1	A	310	ILE	2.1
1	B	317	GLU	2.1
1	B	399	GLU	2.1
1	B	52	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	233	ILE	2.1
1	A	262	LEU	2.1
1	B	344	ILE	2.1
1	D	377	GLY	2.1
1	B	37	SER	2.1
1	B	236	LYS	2.1
1	B	241	ASP	2.1
1	D	299	HIS	2.1
1	D	328	ASP	2.1
1	A	148	VAL	2.1
1	C	70	VAL	2.1
1	B	36	PHE	2.1
1	C	234	GLY	2.1
1	B	361	ARG	2.1
1	D	128	ARG	2.1
1	B	414	THR	2.0
1	D	70	VAL	2.0
1	B	156	TRP	2.0
1	B	338	TRP	2.0
1	B	271	SER	2.0
1	A	244	GLN	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 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.