



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 03:28 pm GMT

PDB ID : 4L23  
Title : Crystal Structure of p110alpha complexed with niSH2 of p85alpha and PI-103  
Authors : Zhang, J.; Zhao, Y.L.; Chen, Y.Y.; Huang, M.; Jiang, F.  
Deposited on : 2013-06-04  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

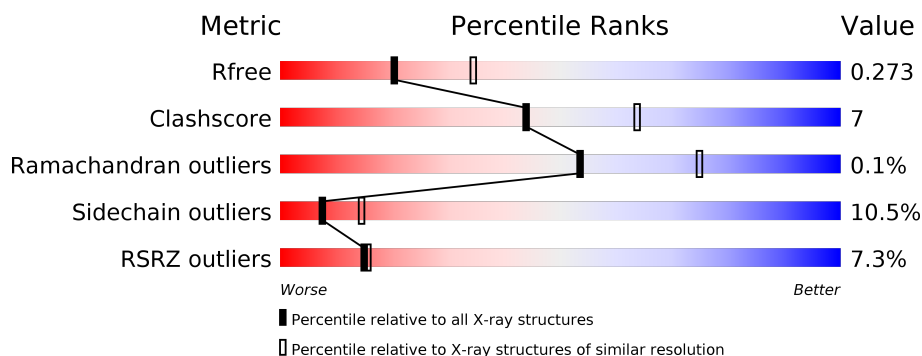
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	1068	
2	B	324	

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
4	SO4	B	701	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10928 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	0	0
			8280	5298	1410	1504	68			

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	277	Total	C	N	O	S	0	0	0
			2354	1474	420	452	8			

There are 26 discrepancies between the modelled and reference sequences:

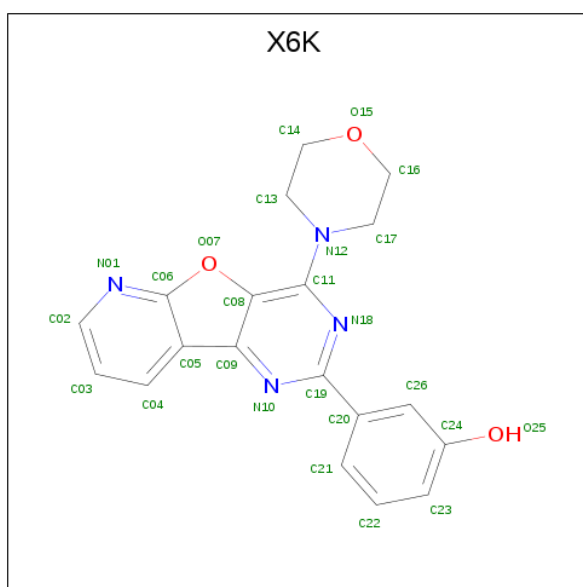
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	MET	-	EXPRESSION TAG	UNP P27986
B	293	SER	-	EXPRESSION TAG	UNP P27986
B	294	TYR	-	EXPRESSION TAG	UNP P27986
B	295	TYR	-	EXPRESSION TAG	UNP P27986
B	296	HIS	-	EXPRESSION TAG	UNP P27986
B	297	HIS	-	EXPRESSION TAG	UNP P27986
B	298	HIS	-	EXPRESSION TAG	UNP P27986
B	299	HIS	-	EXPRESSION TAG	UNP P27986
B	300	HIS	-	EXPRESSION TAG	UNP P27986
B	301	HIS	-	EXPRESSION TAG	UNP P27986
B	302	ASP	-	EXPRESSION TAG	UNP P27986
B	303	TYR	-	EXPRESSION TAG	UNP P27986
B	304	ASP	-	EXPRESSION TAG	UNP P27986
B	305	ILE	-	EXPRESSION TAG	UNP P27986
B	306	PRO	-	EXPRESSION TAG	UNP P27986
B	307	THR	-	EXPRESSION TAG	UNP P27986
B	308	THR	-	EXPRESSION TAG	UNP P27986
B	309	GLU	-	EXPRESSION TAG	UNP P27986
B	310	ASN	-	EXPRESSION TAG	UNP P27986

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Chain	Residue	Modelled	Actual	Comment	Reference
B	311	LEU	-	EXPRESSION TAG	UNP P27986
B	312	TYR	-	EXPRESSION TAG	UNP P27986
B	313	PHE	-	EXPRESSION TAG	UNP P27986
B	314	GLN	-	EXPRESSION TAG	UNP P27986
B	315	SER	-	EXPRESSION TAG	UNP P27986
B	316	ILE	-	EXPRESSION TAG	UNP P27986
B	317	ALA	-	EXPRESSION TAG	UNP P27986

- Molecule 3 is 3-(4-MORPHOLIN-4-YLPYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL)PHENOL (three-letter code: X6K) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

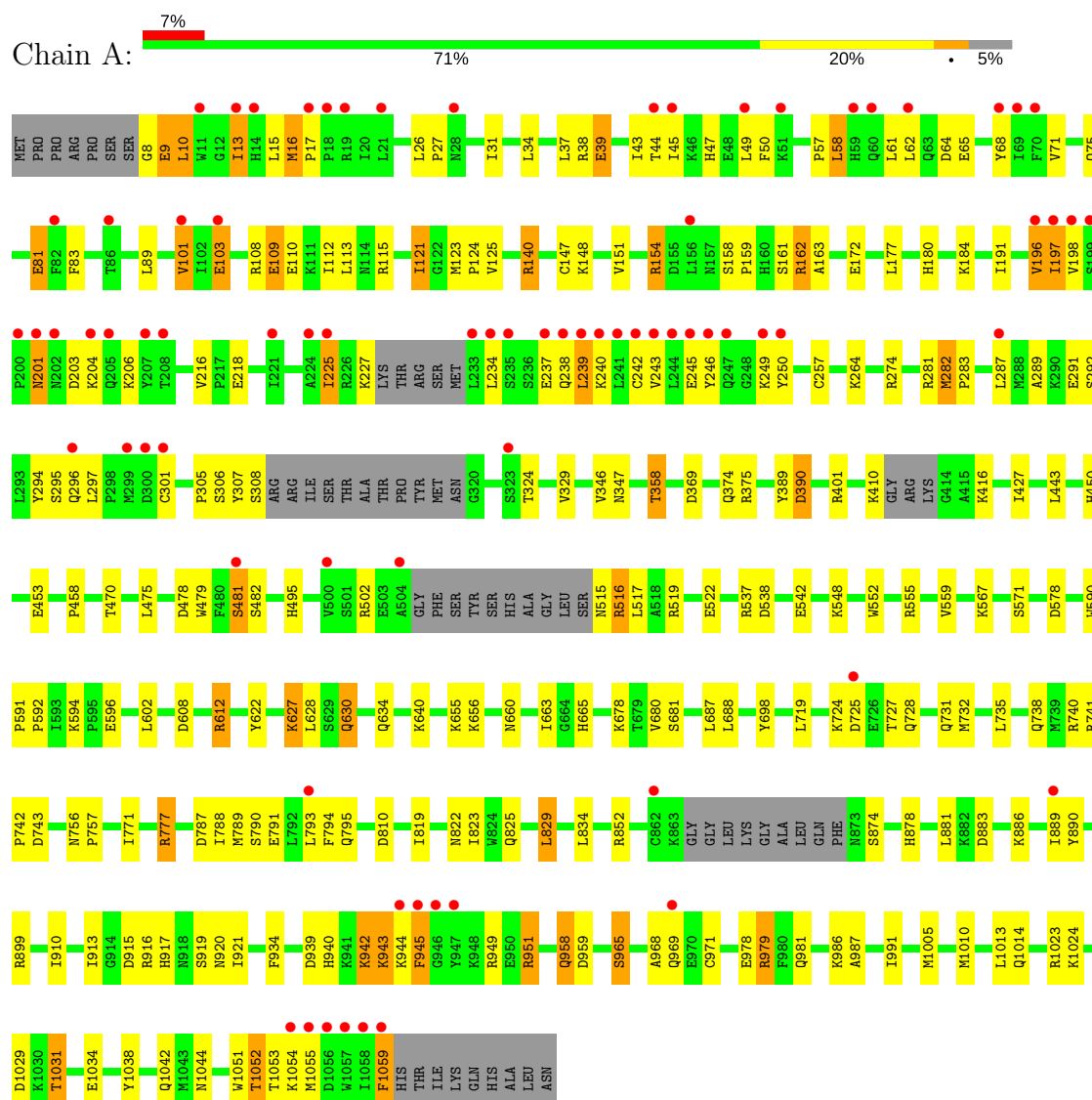
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	203	Total 203	O 203	0	0
6	B	49	Total 49	O 49	0	0

### 3 Residue-property plots

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.

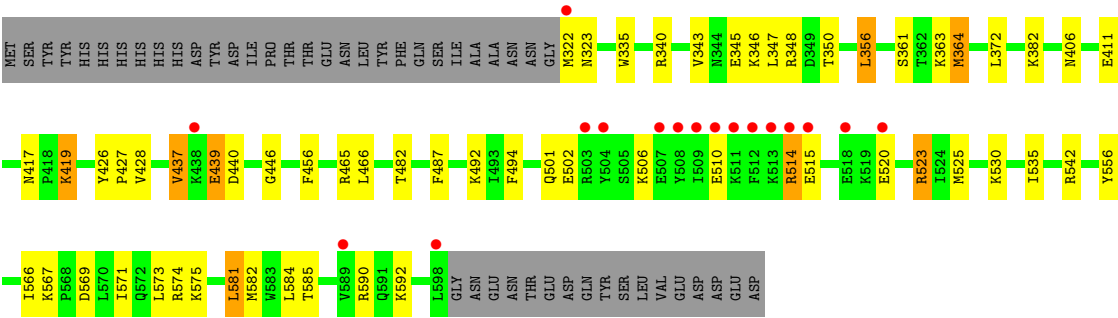
- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.63Å 136.38Å 151.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.98 – 2.50 39.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.98-2.50) 98.0 (39.50-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.215 , 0.273 0.215 , 0.273	Depositor DCC
$R_{free}$ test set	2606 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: GOL, X6K, 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	0.24	0/8464	0.44	0/11441
2	B	0.23	0/2394	0.43	0/3207
All	All	0.24	0/10858	0.44	0/14648

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	8280	0	8258	125	0
2	B	2354	0	2330	32	0
3	A	26	0	15	1	0
4	A	5	0	0	0	0
4	B	5	0	0	4	0
5	B	6	0	8	1	0
6	A	203	0	0	6	0
6	B	49	0	0	1	0
All	All	10928	0	10611	153	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 (153) 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:940:HIS:O	1:A:943:LYS:NZ	2.16	0.77
1:A:958:GLN:NE2	1:A:971:CYS:SG	2.60	0.74
1:A:913:ILE:O	1:A:951:ARG:NH2	2.22	0.72
1:A:981:GLN:NE2	1:A:1051:TRP:O	2.21	0.72
1:A:537:ARG:O	1:A:567:LYS:NZ	2.22	0.72
1:A:64:ASP:O	6:A:1347:HOH:O	2.08	0.71
1:A:154:ARG:HB2	1:A:162:ARG:HH12	1.55	0.70
2:B:382:LYS:NZ	4:B:701:SO4:O3	2.23	0.69
1:A:1044:ASN:ND2	1:A:1052:THR:O	2.27	0.68
2:B:437:VAL:HG23	2:B:439:GLU:HG3	1.74	0.68
1:A:829:LEU:HD11	1:A:986:LYS:HB3	1.77	0.66
1:A:242:CYS:O	1:A:246:TYR:N	2.25	0.64
1:A:1031:THR:HG22	1:A:1034:GLU:H	1.60	0.64
1:A:8:GLY:O	1:A:75:GLN:NE2	2.31	0.64
1:A:949:ARG:NH2	6:A:1273:HOH:O	2.31	0.63
1:A:57:PRO:HG3	2:B:523:ARG:HB2	1.80	0.63
2:B:343:VAL:HG13	2:B:356:LEU:HD21	1.80	0.62
1:A:630:GLN:NE2	6:A:1280:HOH:O	2.33	0.62
1:A:453:GLU:OE1	2:B:574:ARG:NH2	2.33	0.62
1:A:917:HIS:H	1:A:920:ASN:HB2	1.64	0.61
1:A:450:HIS:O	1:A:1014:GLN:NE2	2.33	0.59
1:A:108:ARG:NH1	1:A:109:GLU:OE2	2.35	0.59
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.84	0.59
2:B:335:TRP:CZ3	2:B:582:MET:HE2	2.38	0.59
1:A:878:HIS:NE2	1:A:890:TYR:OH	2.30	0.58
1:A:250:TYR:HD1	1:A:289:ALA:HA	1.70	0.57
1:A:495:HIS:NE2	1:A:578:ASP:OD1	2.31	0.57
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.87	0.56
1:A:148:LYS:HA	1:A:151:VAL:HG22	1.88	0.56
1:A:678:LYS:HA	1:A:681:SER:HB2	1.87	0.56
1:A:965:SER:HB3	1:A:968:ALA:HB3	1.88	0.56
1:A:27:PRO:HD3	1:A:101:VAL:HG22	1.87	0.55
1:A:201:ASN:HD21	1:A:203:ASP:HB3	1.70	0.55
1:A:628:LEU:HD23	1:A:663:ILE:HD13	1.89	0.55
1:A:596:GLU:OE2	1:A:627:LYS:NZ	2.40	0.55
2:B:340:ARG:NH2	4:B:701:SO4:O4	2.36	0.54
1:A:410:LYS:NZ	2:B:569:ASP:OD1	2.28	0.54
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.09	0.53
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.89	0.53
1:A:225:ILE:HD11	1:A:243:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HD12	1:A:688:LEU:HB3	1.90	0.52
1:A:45:ILE:HD11	1:A:89:LEU:HD12	1.90	0.52
1:A:819:ILE:O	1:A:823:ILE:HG12	2.09	0.52
1:A:913:ILE:HD13	1:A:934:PHE:HD1	1.75	0.52
1:A:515:ASN:CG	1:A:516:ARG:H	2.13	0.52
1:A:238:GLN:O	1:A:240:LYS:N	2.43	0.52
2:B:361:SER:HB2	2:B:364:MET:HG3	1.91	0.52
1:A:34:LEU:HD13	1:A:49:LEU:HD12	1.92	0.51
1:A:943:LYS:C	1:A:945:PHE:H	2.14	0.51
1:A:538:ASP:OD2	1:A:1023:ARG:NH1	2.44	0.51
1:A:196:VAL:HG13	1:A:287:LEU:HB3	1.93	0.51
1:A:305:PRO:O	1:A:308:SER:OG	2.27	0.51
1:A:71:VAL:HG22	1:A:81:GLU:HB3	1.94	0.50
1:A:291:GLU:O	1:A:295:SER:OG	2.27	0.50
1:A:68:TYR:HB3	1:A:101:VAL:HG23	1.94	0.49
2:B:514:ARG:O	2:B:515:GLU:HG2	2.12	0.49
2:B:347:LEU:O	2:B:350:THR:OG1	2.25	0.49
1:A:416:LYS:NZ	6:A:1314:HOH:O	2.46	0.49
2:B:382:LYS:NZ	4:B:701:SO4:S	2.85	0.49
1:A:917:HIS:CE1	1:A:919:SER:HB2	2.48	0.49
1:A:1053:THR:OG1	1:A:1054:LYS:N	2.46	0.48
1:A:552:TRP:O	1:A:555:ARG:NH1	2.46	0.48
1:A:9:GLU:OE1	1:A:38:ARG:NH2	2.46	0.48
1:A:140:ARG:HH11	1:A:140:ARG:HG3	1.77	0.48
1:A:374:GLN:NE2	6:A:1369:HOH:O	2.46	0.48
1:A:121:ILE:HG22	1:A:123:MET:HG2	1.97	0.47
1:A:915:ASP:O	1:A:920:ASN:ND2	2.47	0.47
2:B:571:ILE:HG22	2:B:575:LYS:HD2	1.97	0.47
1:A:1053:THR:HG23	1:A:1055:MET:H	1.79	0.47
1:A:719:LEU:HD11	1:A:735:LEU:HD13	1.96	0.47
1:A:390:ASP:OD1	1:A:390:ASP:N	2.44	0.47
1:A:548:LYS:HG2	1:A:571:SER:HA	1.97	0.47
1:A:665:HIS:ND1	1:A:698:TYR:OH	2.43	0.47
1:A:68:TYR:CE1	1:A:103:GLU:HG2	2.50	0.47
1:A:180:HIS:O	1:A:184:LYS:HG3	2.15	0.46
1:A:788:ILE:HD12	1:A:789:MET:HG2	1.96	0.46
1:A:537:ARG:NH1	1:A:542:GLU:O	2.39	0.46
1:A:64:ASP:OD1	1:A:65:GLU:N	2.48	0.46
1:A:943:LYS:H	1:A:943:LYS:HG3	1.57	0.46
2:B:335:TRP:HZ3	2:B:582:MET:HE2	1.80	0.46
1:A:83:PHE:HB2	1:A:112:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:GLY:HA2	2:B:584:LEU:HD11	1.97	0.46
1:A:910:ILE:HD13	1:A:991:ILE:HG21	1.97	0.46
1:A:401:ARG:NH2	1:A:458:PRO:O	2.37	0.46
1:A:140:ARG:HD2	1:A:307:TYR:CE2	2.50	0.46
1:A:427:ILE:HD11	1:A:443:LEU:HD22	1.98	0.46
2:B:345:GLU:OE2	2:B:348:ARG:NH1	2.48	0.46
1:A:218:GLU:HG2	6:A:1326:HOH:O	2.16	0.45
1:A:1059:PHE:CD2	1:A:1059:PHE:N	2.84	0.45
1:A:943:LYS:HB2	1:A:943:LYS:HE2	1.82	0.45
2:B:348:ARG:NH1	6:B:817:HOH:O	2.49	0.45
1:A:899:ARG:NH2	1:A:979:ARG:HH22	2.15	0.45
1:A:602:LEU:O	1:A:612:ARG:NH2	2.50	0.45
1:A:731:GLN:OE1	1:A:777:ARG:NE	2.50	0.45
1:A:45:ILE:O	1:A:49:LEU:HB2	2.16	0.44
1:A:50:PHE:HB2	1:A:65:GLU:OE1	2.17	0.44
1:A:1059:PHE:N	1:A:1059:PHE:HD2	2.16	0.44
2:B:520:GLU:HA	2:B:523:ARG:HD3	1.98	0.44
1:A:590:TRP:HA	1:A:591:PRO:HD3	1.88	0.44
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.87	0.44
1:A:197:ILE:H	1:A:197:ILE:HG12	1.51	0.43
1:A:31:ILE:O	2:B:530:LYS:NZ	2.48	0.43
1:A:787:ASP:O	1:A:790:SER:HB3	2.17	0.43
1:A:791:GLU:HA	1:A:795:GLN:HG3	2.00	0.43
1:A:479:TRP:CZ3	1:A:481:SER:HA	2.53	0.43
2:B:567:LYS:O	2:B:571:ILE:HG12	2.18	0.43
1:A:140:ARG:HG3	1:A:140:ARG:NH1	2.33	0.43
2:B:417:ASN:OD1	2:B:419:LYS:HG2	2.19	0.43
1:A:50:PHE:HZ	1:A:68:TYR:HD2	1.66	0.43
1:A:1010:MET:HB2	1:A:1010:MET:HE3	1.88	0.42
1:A:939:ASP:O	1:A:942:LYS:HB3	2.19	0.42
1:A:987:ALA:O	1:A:991:ILE:HG12	2.19	0.42
1:A:741:ARG:HA	1:A:742:PRO:HD3	1.93	0.42
1:A:756:ASN:HA	1:A:757:PRO:HD2	1.87	0.42
1:A:732:MET:SD	1:A:771:ILE:HG13	2.60	0.42
1:A:358:THR:HG21	1:A:389:TYR:OH	2.19	0.42
1:A:883:ASP:HA	1:A:886:LYS:HD3	2.01	0.42
2:B:590:ARG:HG2	2:B:592:LYS:HB2	2.01	0.42
2:B:382:LYS:NZ	4:B:701:SO4:O2	2.52	0.42
1:A:13:ILE:HG23	1:A:15:LEU:N	2.35	0.42
1:A:47:HIS:HA	1:A:65:GLU:OE1	2.19	0.42
1:A:592:PRO:HB2	1:A:622:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:LYS:O	2:B:510:GLU:HB2	2.19	0.42
1:A:656:LYS:HD3	1:A:656:LYS:HA	1.74	0.41
1:A:16:MET:HA	1:A:17:PRO:HD3	1.95	0.41
1:A:50:PHE:CZ	1:A:68:TYR:HD2	2.37	0.41
1:A:58:LEU:HA	1:A:58:LEU:HD12	1.88	0.41
1:A:660:ASN:HB3	1:A:663:ILE:HD12	2.02	0.41
1:A:172:GLU:HG3	1:A:274:ARG:CZ	2.50	0.41
2:B:494:PHE:HB3	2:B:535:ILE:HG12	2.02	0.41
1:A:26:LEU:HD13	1:A:62:LEU:HD11	2.03	0.41
1:A:608:ASP:O	1:A:612:ARG:HG3	2.21	0.41
1:A:793:LEU:HG	1:A:794:PHE:CD1	2.56	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.85	0.41
1:A:810:ASP:OD2	3:A:1101:X6K:O25	2.39	0.41
1:A:180:HIS:HE1	1:A:825:GLN:O	2.04	0.41
2:B:346:LYS:HD3	2:B:428:VAL:HG11	2.03	0.41
1:A:634:GLN:HG3	1:A:1005:MET:SD	2.60	0.41
1:A:123:MET:HA	1:A:124:PRO:HD3	1.86	0.41
1:A:159:PRO:HG2	1:A:294:TYR:CD2	2.56	0.41
1:A:16:MET:O	1:A:38:ARG:HD2	2.21	0.41
2:B:466:LEU:HD12	2:B:566:ILE:HD12	2.01	0.41
1:A:1024:LYS:HB3	1:A:1024:LYS:HE3	1.94	0.41
1:A:282:MET:HA	1:A:283:PRO:HD3	1.92	0.41
2:B:323:ASN:HB3	2:B:406:ASN:ND2	2.36	0.41
1:A:1023:ARG:NH2	1:A:1029:ASP:OD2	2.54	0.41
2:B:456:PHE:HB2	2:B:573:LEU:HB3	2.03	0.41
1:A:108:ARG:O	1:A:112:ILE:HG12	2.21	0.40
1:A:147:CYS:O	1:A:151:VAL:HG13	2.21	0.40
1:A:39:GLU:OE1	1:A:741:ARG:NH2	2.54	0.40
2:B:581:LEU:HD22	2:B:581:LEU:HA	1.78	0.40
2:B:426:TYR:HA	2:B:427:PRO:HD2	1.96	0.40
2:B:556:TYR:CD1	5:B:702:GOL:H11	2.56	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	1002/1068 (94%)	975 (97%)	26 (3%)	1 (0%)	53	75
2	B	275/324 (85%)	271 (98%)	4 (2%)	0	100	100
All	All	1277/1392 (92%)	1246 (98%)	30 (2%)	1 (0%)	53	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	LEU

### 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	924/974 (95%)	822 (89%)	102 (11%)	7	13
2	B	258/301 (86%)	236 (92%)	22 (8%)	12	22
All	All	1182/1275 (93%)	1058 (90%)	124 (10%)	7	14

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	10	LEU
1	A	13	ILE
1	A	16	MET
1	A	37	LEU
1	A	39	GLU
1	A	43	ILE
1	A	44	THR
1	A	58	LEU
1	A	61	LEU
1	A	81	GLU
1	A	101	VAL

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	109	GLU
1	A	110	GLU
1	A	113	LEU
1	A	115	ARG
1	A	121	ILE
1	A	125	VAL
1	A	140	ARG
1	A	154	ARG
1	A	158	SER
1	A	161	SER
1	A	162	ARG
1	A	191	ILE
1	A	196	VAL
1	A	197	ILE
1	A	198	VAL
1	A	201	ASN
1	A	204	LYS
1	A	206	LYS
1	A	216	VAL
1	A	225	ILE
1	A	227	LYS
1	A	234	LEU
1	A	237	GLU
1	A	239	LEU
1	A	245	GLU
1	A	249	LYS
1	A	257	CYS
1	A	264	LYS
1	A	281	ARG
1	A	282	MET
1	A	292	SER
1	A	296	GLN
1	A	301	CYS
1	A	306	SER
1	A	324	THR
1	A	329	VAL
1	A	346	VAL
1	A	347	ASN
1	A	358	THR
1	A	369	ASP
1	A	375	ARG

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Mol	Chain	Res	Type
1	A	390	ASP
1	A	470	THR
1	A	475	LEU
1	A	478	ASP
1	A	481	SER
1	A	482	SER
1	A	502	ARG
1	A	516	ARG
1	A	517	LEU
1	A	519	ARG
1	A	522	GLU
1	A	559	VAL
1	A	594	LYS
1	A	612	ARG
1	A	627	LYS
1	A	630	GLN
1	A	655	LYS
1	A	687	LEU
1	A	724	LYS
1	A	725	ASP
1	A	727	THR
1	A	728	GLN
1	A	738	GLN
1	A	740	ARG
1	A	743	ASP
1	A	777	ARG
1	A	822	ASN
1	A	829	LEU
1	A	834	LEU
1	A	852	ARG
1	A	874	SER
1	A	881	LEU
1	A	889	ILE
1	A	942	LYS
1	A	943	LYS
1	A	944	LYS
1	A	945	PHE
1	A	951	ARG
1	A	958	GLN
1	A	959	ASP
1	A	965	SER
1	A	969	GLN

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Mol	Chain	Res	Type
1	A	978	GLU
1	A	979	ARG
1	A	1013	LEU
1	A	1031	THR
1	A	1052	THR
1	A	1059	PHE
2	B	322	MET
2	B	356	LEU
2	B	363	LYS
2	B	364	MET
2	B	372	LEU
2	B	411	GLU
2	B	419	LYS
2	B	437	VAL
2	B	439	GLU
2	B	440	ASP
2	B	465	ARG
2	B	482	THR
2	B	487	PHE
2	B	492	LYS
2	B	501	GLN
2	B	502	GLU
2	B	514	ARG
2	B	523	ARG
2	B	525	MET
2	B	542	ARG
2	B	581	LEU
2	B	585	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	958	GLN
2	B	453	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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
3	X6K	A	1101	-	26,30,30	1.17	2 (7%)	30,43,43	1.89	9 (30%)
4	SO4	A	1102	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	B	701	-	4,4,4	0.17	0	6,6,6	0.09	0
5	GOL	B	702	-	5,5,5	0.39	0	5,5,5	0.26	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
3	X6K	A	1101	-	-	0/8/16/16	0/5/5/5
4	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
4	SO4	B	701	-	-	0/0/0/0	0/0/0/0
5	GOL	B	702	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	X6K	C05-C06	2.66	1.48	1.42
3	A	1101	X6K	C11-N18	2.82	1.36	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	X6K	N10-C19-N18	-4.36	122.49	126.17
3	A	1101	X6K	C03-C04-C05	-4.14	113.71	120.83
3	A	1101	X6K	C05-C06-N01	-3.03	119.89	124.94
3	A	1101	X6K	C16-C17-N12	-2.77	104.90	109.92
3	A	1101	X6K	C14-C13-N12	-2.58	105.24	109.92
3	A	1101	X6K	C20-C19-N10	2.17	120.42	116.32
3	A	1101	X6K	C04-C03-C02	2.28	121.92	118.92
3	A	1101	X6K	C04-C05-C06	2.44	123.14	118.36
3	A	1101	X6K	C11-N18-C19	4.09	124.62	116.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	X6K	1	0
4	B	701	SO4	4	0
5	B	702	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1014/1068 (94%)	0.39	77 (7%) 14 14	26, 47, 89, 117	0
2	B	277/324 (85%)	0.30	17 (6%) 21 22	33, 52, 91, 109	0
All	All	1291/1392 (92%)	0.37	94 (7%) 15 16	26, 48, 90, 117	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	LEU	10.8
1	A	238	GLN	6.7
1	A	205	GLN	6.4
1	A	197	ILE	6.0
1	A	233	LEU	5.3
1	A	504	ALA	5.2
1	A	244	LEU	5.0
2	B	508	TYR	5.0
1	A	1059	PHE	5.0
1	A	250	TYR	5.0
1	A	198	VAL	4.9
2	B	504	TYR	4.9
1	A	14	HIS	4.8
1	A	199	SER	4.8
1	A	246	TYR	4.7
1	A	944	LYS	4.6
1	A	946	GLY	4.6
1	A	500	VAL	4.5
1	A	207	TYR	4.5
1	A	237	GLU	4.5
1	A	245	GLU	4.4
2	B	322	MET	4.4
1	A	202	ASN	4.4
2	B	514	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	438	LYS	4.4
1	A	323	SER	4.3
1	A	249	LYS	4.2
1	A	243	VAL	4.1
1	A	1056	ASP	4.0
1	A	62	LEU	3.9
1	A	481	SER	3.9
2	B	511	LYS	3.8
1	A	1058	ILE	3.8
2	B	507	GLU	3.7
1	A	224	ALA	3.7
1	A	945	PHE	3.7
1	A	204	LYS	3.7
2	B	515	GLU	3.6
1	A	28	ASN	3.6
1	A	68	TYR	3.6
1	A	1057	TRP	3.6
2	B	512	PHE	3.5
1	A	239	LEU	3.4
1	A	196	VAL	3.4
1	A	225	ILE	3.4
1	A	240	LYS	3.4
1	A	17	PRO	3.2
1	A	49	LEU	3.2
1	A	13	ILE	3.2
1	A	947	TYR	3.1
1	A	200	PRO	3.1
2	B	510	GLU	3.0
1	A	1054	LYS	3.0
1	A	18	PRO	3.0
1	A	201	ASN	3.0
1	A	82	PHE	2.9
1	A	221	ILE	2.9
2	B	513	LYS	2.8
1	A	69	ILE	2.8
1	A	1055	MET	2.8
1	A	156	LEU	2.8
1	A	969	GLN	2.7
2	B	520	GLU	2.7
1	A	234	LEU	2.7
1	A	247	GLN	2.7
1	A	862	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	19	ARG	2.6
1	A	300	ASP	2.6
1	A	60	GLN	2.6
2	B	509	ILE	2.6
2	B	503	ARG	2.5
1	A	103	GLU	2.5
2	B	518	GLU	2.5
1	A	235	SER	2.5
1	A	45	ILE	2.5
1	A	208	THR	2.4
1	A	242	CYS	2.4
1	A	59	HIS	2.3
1	A	21	LEU	2.3
1	A	101	VAL	2.3
2	B	598	LEU	2.3
1	A	301	CYS	2.3
1	A	70	PHE	2.2
1	A	889	ILE	2.2
1	A	287	LEU	2.2
1	A	51	LYS	2.1
1	A	11	TRP	2.1
1	A	86	THR	2.1
1	A	793	LEU	2.1
1	A	725	ASP	2.1
1	A	296	GLN	2.1
2	B	589	VAL	2.1
1	A	299	MET	2.1
1	A	44	THR	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	X6K	A	1101	26/26	0.91	0.18	28,36,42,45	0
4	SO4	A	1102	5/5	0.92	0.17	61,66,79,79	0
5	GOL	B	702	6/6	0.96	0.16	35,38,42,43	0
4	SO4	B	701	5/5	0.97	0.15	46,50,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.