



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:52 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

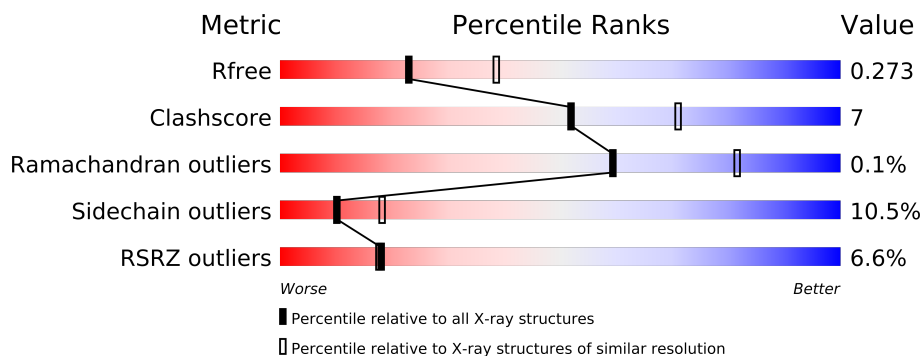
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10928 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

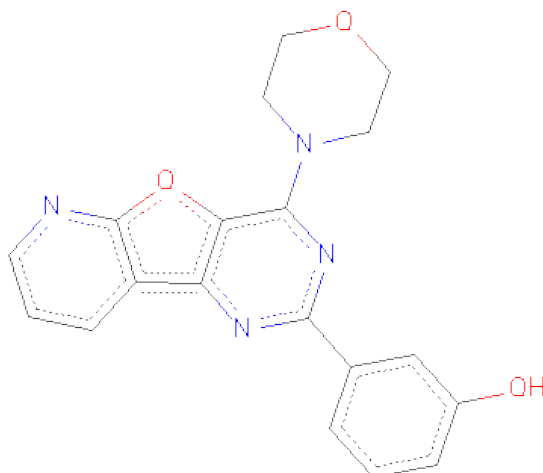
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	MET	-	EXPRESSION TAG	UNP P27986
B	293	SER	-	EXPRESSION TAG	UNP P27986
B	294	TYR	-	EXPRESSION TAG	UNP P27986
B	295	TYR	-	EXPRESSION TAG	UNP P27986
B	296	HIS	-	EXPRESSION TAG	UNP P27986
B	297	HIS	-	EXPRESSION TAG	UNP P27986
B	298	HIS	-	EXPRESSION TAG	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: C₁₉H₁₆N₄O₃).



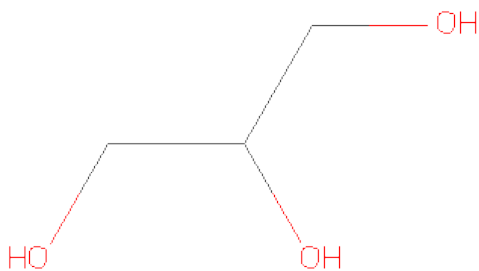
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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		

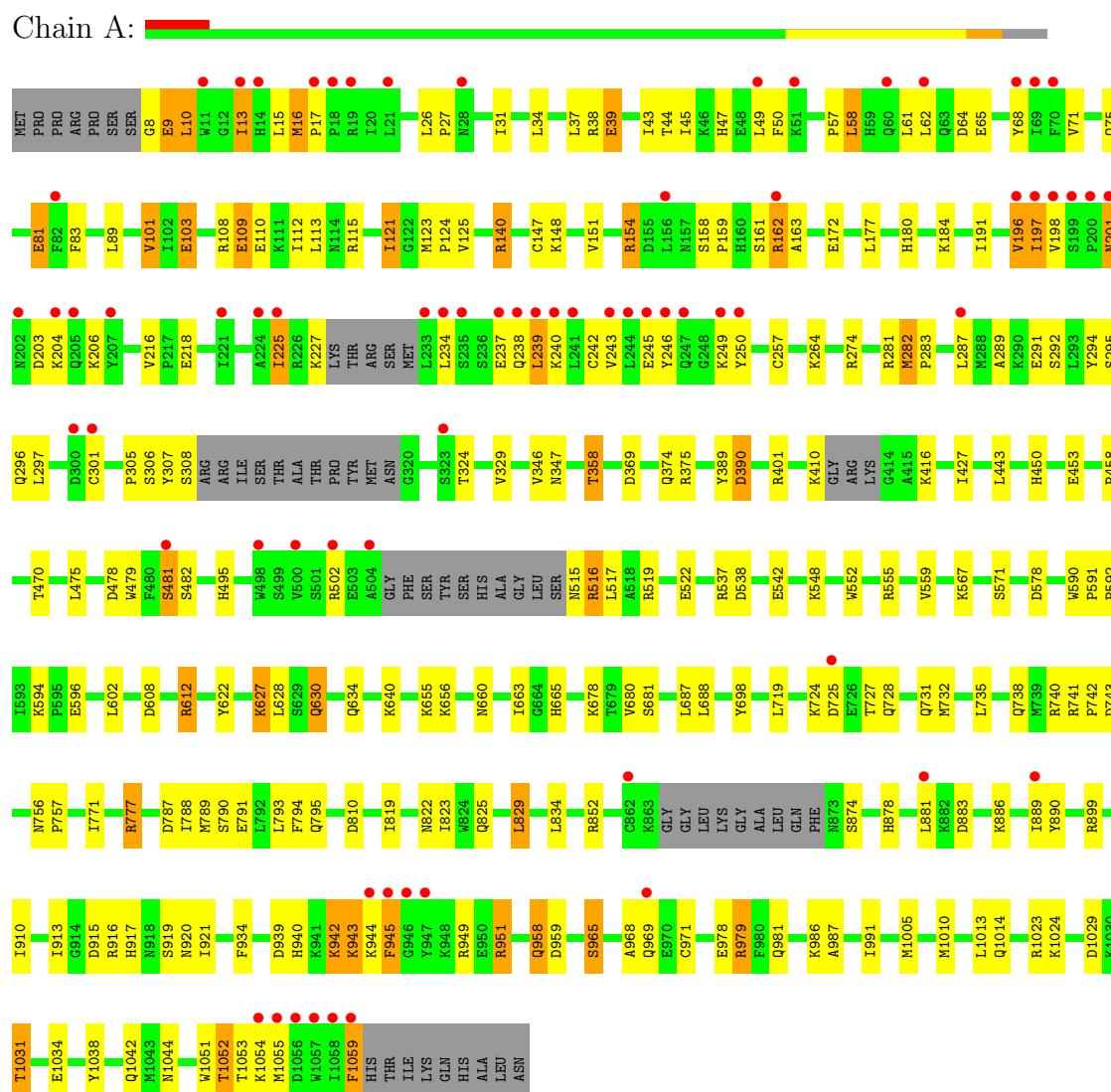
- Molecule 6 is water.

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

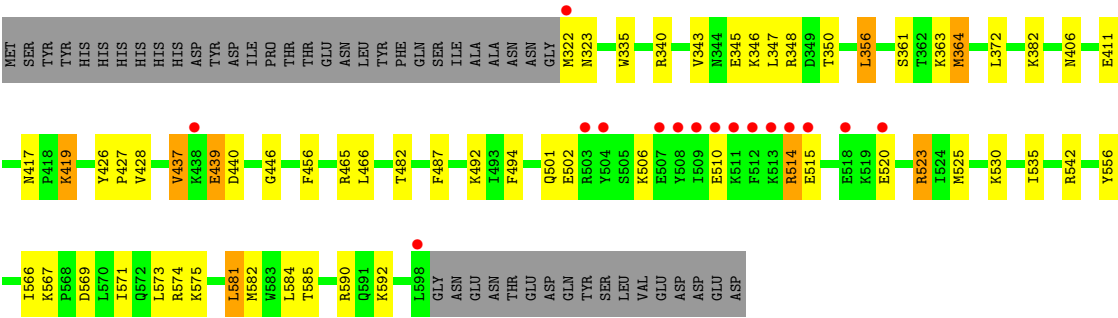
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.273 0.215 , 0.273	Depositor DCC
R_{free} test set	2607 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51036 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10928	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 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:981:GLN:NE2	1:A:1051:TRP:O	2.21	0.72
1:A:913:ILE:O	1:A:951:ARG:NH2	2.22	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:453:GLU:OE1	2:B:574:ARG:NH2	2.33	0.62
1:A:630:GLN:NE2	6:A:1280:HOH:O	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:225:ILE:HD11	1:A:243:VAL:HG12	1.90	0.52
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:913:ILE:HD13	1:A:934:PHE:HD1	1.75	0.52
1:A:819:ILE:O	1:A:823:ILE:HG12	2.09	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:943:LYS:C	1:A:945:PHE:H	2.14	0.51
1:A:34:LEU:HD13	1:A:49:LEU:HD12	1.92	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
2:B:382:LYS:NZ	4:B:701:SO4:S	2.85	0.49
1:A:416:LYS:NZ	6:A:1314:HOH:O	2.46	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:915:ASP:O	1:A:920:ASN:ND2	2.47	0.47
1:A:121:ILE:HG22	1:A:123:MET:HG2	1.97	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:788:ILE:HD12	1:A:789:MET:HG2	1.96	0.46
1:A:180:HIS:O	1:A:184:LYS:HG3	2.15	0.46
1:A:537:ARG:NH1	1:A:542:GLU:O	2.39	0.46
1:A:943:LYS:HG3	1:A:943:LYS:H	1.57	0.46
1:A:64:ASP:OD1	1:A:65:GLU:N	2.48	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	Distance(Å)	Clash(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: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:1059:PHE:CD2	1:A:1059:PHE:N	2.84	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
2:B:520:GLU:HA	2:B:523:ARG:HD3	1.98	0.44
1:A:1059:PHE:N	1:A:1059:PHE:HD2	2.16	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:787:ASP:O	1:A:790:SER:HB3	2.17	0.43
1:A:31:ILE:O	2:B:530:LYS:NZ	2.48	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:987:ALA:O	1:A:991:ILE:HG12	2.19	0.42
1:A:939:ASP:O	1:A:942:LYS:HB3	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:883:ASP:HA	1:A:886:LYS:HD3	2.01	0.42
1:A:358:THR:HG21	1:A:389:TYR:OH	2.19	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:47:HIS:HA	1:A:65:GLU:OE1	2.19	0.42
2:B:506:LYS:O	2:B:510:GLU:HB2	2.19	0.42
1:A:13:ILE:HG23	1:A:15:LEU:N	2.35	0.42
1:A:592:PRO:HB2	1:A:622:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:656:LYS:HD3	1:A:656:LYS:HA	1.74	0.41
1:A:50:PHE:CZ	1:A:68:TYR:HD2	2.37	0.41
1:A:660:ASN:HB3	1:A:663:ILE:HD12	2.02	0.41
1:A:16:MET:HA	1:A:17:PRO:HD3	1.95	0.41
1:A:58:LEU:HA	1:A:58:LEU:HD12	1.88	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:180:HIS:HE1	1:A:825:GLN:O	2.04	0.41
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.85	0.41
2:B:346:LYS:HD3	2:B:428:VAL:HG11	2.03	0.41
1:A:810:ASP:OD2	3:A:1101:X6K:O25	2.39	0.41
1:A:123:MET:HA	1:A:124:PRO:HD3	1.86	0.41
1:A:16:MET:O	1:A:38:ARG:HD2	2.21	0.41
1:A:159:PRO:HG2	1:A:294:TYR:CD2	2.56	0.41
1:A:634:GLN:HG3	1:A:1005:MET:SD	2.60	0.41
2:B:466:LEU:HD12	2:B:566:ILE:HD12	2.01	0.41
1:A:1024:LYS:HE3	1:A:1024:LYS:HB3	1.94	0.41
2:B:323:ASN:HB3	2:B:406:ASN:ND2	2.36	0.41
1:A:282:MET:HA	1:A:283:PRO:HD3	1.92	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%)	59	81
2	B	275/324 (85%)	271 (98%)	4 (2%)	0	100	100
All	All	1277/1392 (92%)	1246 (98%)	30 (2%)	1 (0%)	59	81

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%)	9	16
2	B	258/301 (86%)	236 (92%)	22 (8%)	15	28
All	All	1182/1275 (93%)	1058 (90%)	124 (10%)	10	18

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
1	A	103	GLU
1	A	109	GLU
1	A	110	GLU
1	A	113	LEU

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Mol	Chain	Res	Type
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
1	A	390	ASP
1	A	470	THR
1	A	475	LEU
1	A	478	ASP

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Mol	Chain	Res	Type
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
1	A	978	GLU
1	A	979	ARG
1	A	1013	LEU
1	A	1031	THR

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Mol	Chain	Res	Type
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 chains 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 ⓘ

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	-	28,30,30	1.27	3 (10%)	35,43,43	2.26	14 (40%)
4	SO4	A	1102	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	B	701	-	4,4,4	0.16	0	6,6,6	0.07	0
5	GOL	B	702	-	5,5,5	0.37	0	5,5,5	0.23	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	0/2/5/5
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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	X6K	C19-N10	3.23	1.37	1.32
3	A	1101	X6K	C05-C09	3.06	1.47	1.41
3	A	1101	X6K	C11-N18	2.60	1.36	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	X6K	N10-C19-N18	-5.42	122.49	126.10
3	A	1101	X6K	C11-N18-C19	5.06	124.62	116.16
3	A	1101	X6K	N18-C11-N12	4.92	122.03	116.97
3	A	1101	X6K	C03-C04-C05	-3.97	113.71	120.74
3	A	1101	X6K	C05-C09-C08	-3.22	104.41	108.49
3	A	1101	X6K	C05-C06-N01	-2.90	119.89	124.93
3	A	1101	X6K	C19-N10-C09	2.76	118.23	116.25
3	A	1101	X6K	C20-C19-N10	2.76	120.42	118.06
3	A	1101	X6K	C16-C17-N12	-2.69	104.90	110.05
3	A	1101	X6K	C08-C11-N18	-2.53	114.78	120.67
3	A	1101	X6K	C14-C13-N12	-2.51	105.24	110.05
3	A	1101	X6K	C04-C05-C06	2.44	123.14	118.70
3	A	1101	X6K	O07-C08-C09	2.32	111.31	107.42
3	A	1101	X6K	C04-C03-C02	2.18	121.92	118.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1014/1068 (94%)	0.38	70 (6%)	17 16	26, 47, 89, 117	0
2	B	277/324 (85%)	0.31	16 (5%)	22 23	33, 52, 91, 109	0
All	All	1291/1392 (92%)	0.36	86 (6%)	18 17	26, 48, 90, 117	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	LEU	9.6
1	A	197	ILE	6.1
1	A	205	GLN	6.0
1	A	238	GLN	6.0
1	A	504	ALA	5.7
2	B	508	TYR	5.5
2	B	504	TYR	5.2
1	A	250	TYR	5.0
1	A	944	LYS	4.9
1	A	1059	PHE	4.9
1	A	198	VAL	4.7
1	A	946	GLY	4.7
1	A	207	TYR	4.4
2	B	322	MET	4.4
1	A	244	LEU	4.4
1	A	233	LEU	4.4
1	A	237	GLU	4.3
1	A	246	TYR	4.2
1	A	249	LYS	4.2
1	A	199	SER	4.1
1	A	500	VAL	4.0
2	B	438	LYS	4.0
2	B	512	PHE	3.9
1	A	225	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1058	ILE	3.7
1	A	28	ASN	3.7
1	A	323	SER	3.7
1	A	204	LYS	3.6
1	A	945	PHE	3.6
1	A	224	ALA	3.6
1	A	14	HIS	3.5
1	A	947	TYR	3.5
1	A	245	GLU	3.5
1	A	49	LEU	3.5
1	A	481	SER	3.5
1	A	62	LEU	3.5
2	B	509	ILE	3.4
2	B	507	GLU	3.4
1	A	202	ASN	3.4
2	B	511	LYS	3.3
1	A	1057	TRP	3.3
1	A	1056	ASP	3.3
1	A	1054	LYS	3.3
1	A	243	VAL	3.2
2	B	514	ARG	3.1
1	A	13	ILE	3.1
2	B	520	GLU	3.1
1	A	240	LYS	3.1
1	A	68	TYR	3.1
1	A	51	LYS	2.9
2	B	598	LEU	2.8
1	A	287	LEU	2.8
2	B	515	GLU	2.8
1	A	196	VAL	2.7
1	A	235	SER	2.6
1	A	300	ASP	2.6
2	B	513	LYS	2.6
1	A	201	ASN	2.6
1	A	200	PRO	2.6
1	A	19	ARG	2.5
2	B	518	GLU	2.5
1	A	234	LEU	2.5
1	A	17	PRO	2.5
1	A	247	GLN	2.5
1	A	221	ILE	2.5
1	A	498	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	69	ILE	2.4
1	A	889	ILE	2.4
1	A	969	GLN	2.4
1	A	239	LEU	2.4
1	A	18	PRO	2.4
1	A	301	CYS	2.4
1	A	1055	MET	2.4
1	A	725	ASP	2.4
1	A	60	GLN	2.3
2	B	503	ARG	2.3
1	A	156	LEU	2.3
1	A	11	TRP	2.2
2	B	510	GLU	2.2
1	A	862	CYS	2.1
1	A	502	ARG	2.1
1	A	70	PHE	2.1
1	A	21	LEU	2.1
1	A	82	PHE	2.1
1	A	162	ARG	2.0
1	A	881	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	1102	5/5	0.19	1.65	61,66,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	B	702	6/6	0.16	0.59	35,38,42,43	0
3	X6K	A	1101	26/26	0.17	0.34	28,36,42,45	0
4	SO4	B	701	5/5	0.13	-1.21	46,50,54,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.