



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:59 AM GMT

PDB ID : 4L1B
Title : Crystal Structure of p110alpha complexed with niSH2 of p85alpha
Authors : Zhang, J.; Zhao, Y.L.; Chen, Y.Y.; Huang, M.; Jiang, F.
Deposited on : 2013-06-03
Resolution : 2.59 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>

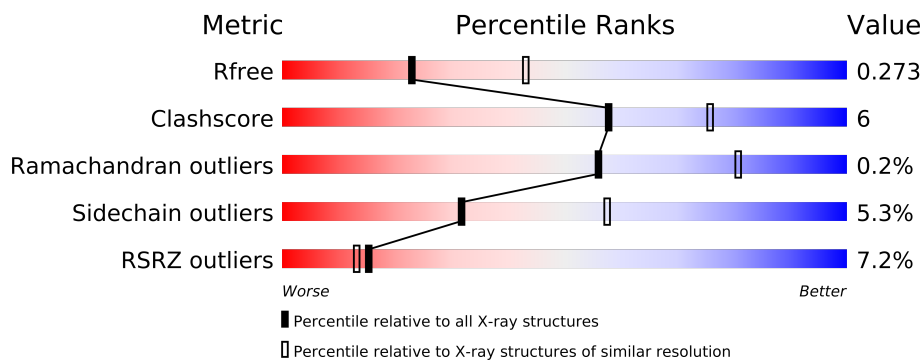
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.59 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	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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 4 unique types of molecules in this entry. The entry contains 10528 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	994	Total	C	N	O	S	0	0	0
			8132	5205	1383	1476	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:

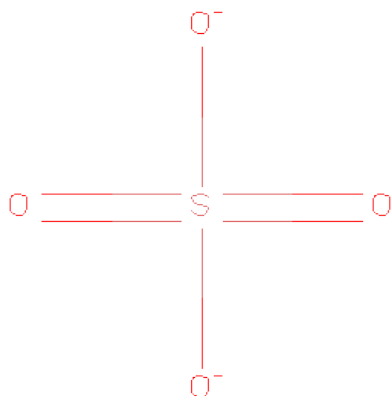
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	MET	-	EXPRESSION TAG	UNP P27986
B	293	SER	-	EXPRESSION TAG	UNP P27986
B	294	TYR	-	EXPRESSION TAG	UNP P27986
B	295	TYR	-	EXPRESSION TAG	UNP P27986
B	296	HIS	-	EXPRESSION TAG	UNP P27986
B	297	HIS	-	EXPRESSION TAG	UNP P27986
B	298	HIS	-	EXPRESSION TAG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

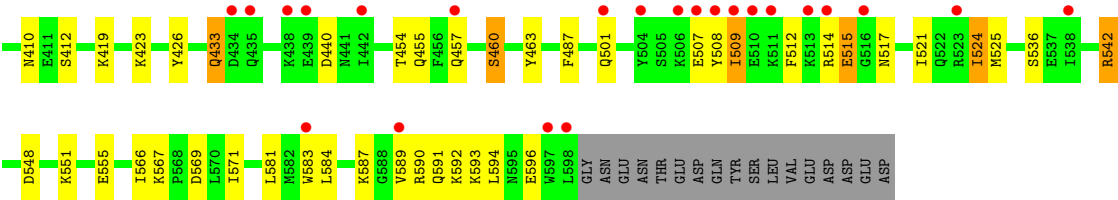
- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	6	Total	O	0	0
			6	6		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.56Å 136.90Å 150.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.59 47.09 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.09-2.59) 95.5 (47.09-2.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.274 0.215 , 0.273	Depositor DCC
R_{free} test set	2217 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46122 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: 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	0.25	0/8316	0.46	0/11242
2	B	0.25	0/2394	0.47	0/3207
All	All	0.25	0/10710	0.46	0/14449

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	8132	0	8110	104	0
2	B	2354	0	2330	31	0
3	B	5	0	0	0	0
4	A	31	0	0	0	0
4	B	6	0	0	0	0
All	All	10528	0	10440	132	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 6.

All (132) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:216:VAL:HG12	1:A:218:GLU:H	1.50	0.76
1:A:917:HIS:H	1:A:920:ASN:HB2	1.55	0.71
2:B:514:ARG:O	2:B:515:GLU:HB3	1.92	0.68
2:B:542:ARG:HH11	2:B:542:ARG:HG2	1.57	0.68
1:A:215:CYS:HB3	1:A:219:GLN:HG3	1.77	0.67
1:A:42:LEU:HD12	1:A:85:GLU:HA	1.78	0.66
1:A:209:LEU:HD21	1:A:223:GLU:HB3	1.78	0.66
1:A:537:ARG:NH1	1:A:543:ILE:HA	2.12	0.65
2:B:512:PHE:HB3	2:B:517:ASN:HB3	1.81	0.62
1:A:410:LYS:NZ	2:B:569:ASP:OD1	2.32	0.62
2:B:366:GLY:HA3	2:B:382:LYS:HD3	1.84	0.60
1:A:537:ARG:O	1:A:567:LYS:NZ	2.33	0.60
1:A:637:GLN:NE2	1:A:674:GLU:OE2	2.27	0.58
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.85	0.58
1:A:594:LYS:HG3	1:A:595:PRO:HD2	1.85	0.57
1:A:121:ILE:HG22	1:A:123:MET:HG2	1.86	0.57
1:A:537:ARG:NH1	1:A:547:GLU:OE1	2.38	0.57
1:A:1044:ASN:HA	1:A:1051:TRP:HB3	1.88	0.56
2:B:507:GLU:HG3	2:B:508:TYR:HD1	1.70	0.56
1:A:937:PHE:HD1	1:A:938:LEU:HG	1.69	0.56
1:A:68:TYR:HB3	1:A:101:VAL:HG23	1.88	0.56
2:B:509:ILE:HD11	2:B:524:ILE:HG21	1.87	0.55
1:A:1039:PHE:CZ	1:A:1043:MET:HE2	2.41	0.55
1:A:895:ASP:OD2	1:A:899:ARG:NH2	2.41	0.54
2:B:542:ARG:NH1	2:B:542:ARG:HG2	2.19	0.54
2:B:392:PHE:CZ	2:B:404:LEU:HD21	2.42	0.54
1:A:69:ILE:HG12	1:A:70:PHE:H	1.72	0.54
1:A:105:VAL:O	1:A:111:LYS:NZ	2.39	0.54
2:B:406:ASN:O	2:B:410:ASN:ND2	2.41	0.53
1:A:596:GLU:HA	1:A:599:MET:HE2	1.90	0.53
2:B:590:ARG:NE	2:B:592:LYS:HB2	2.25	0.52
2:B:433:GLN:HG3	2:B:583:TRP:HD1	1.75	0.51
1:A:199:SER:OG	1:A:201:ASN:ND2	2.43	0.51
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.93	0.51
1:A:717:ASP:O	1:A:721:GLN:HG2	2.11	0.51
1:A:129:ASP:OD1	1:A:140:ARG:NH1	2.43	0.50
1:A:194:ILE:HD13	1:A:209:LEU:HD22	1.93	0.50
2:B:463:TYR:HB2	2:B:566:ILE:HG21	1.93	0.50
1:A:121:ILE:HD12	1:A:688:LEU:HB3	1.93	0.50
1:A:640:LYS:HG2	1:A:680:VAL:HG11	1.93	0.50
1:A:959:ASP:O	1:A:963:VAL:HG23	2.12	0.50
1:A:135:GLU:HG2	1:A:645:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:PRO:HB3	1:A:693:ARG:NH1	2.28	0.49
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.94	0.49
1:A:947:TYR:HD1	1:A:949:ARG:HB3	1.78	0.48
1:A:69:ILE:HG12	1:A:70:PHE:N	2.28	0.48
2:B:551:LYS:O	2:B:555:GLU:HG3	2.13	0.48
1:A:1031:THR:HG23	1:A:1033:GLN:H	1.79	0.48
2:B:365:HIS:O	2:B:382:LYS:HD3	2.14	0.48
2:B:567:LYS:O	2:B:571:ILE:HG12	2.13	0.48
1:A:883:ASP:HA	1:A:886:LYS:HD3	1.96	0.47
1:A:819:ILE:O	1:A:823:ILE:HG12	2.13	0.47
1:A:133:ASP:HA	1:A:134:PRO:HD2	1.78	0.47
1:A:787:ASP:O	1:A:790:SER:HB2	2.15	0.47
1:A:728:GLN:HB2	1:A:729:LYS:HE3	1.97	0.47
1:A:542:GLU:OE1	2:B:340:ARG:HD3	2.15	0.47
2:B:584:LEU:HD22	2:B:589:VAL:HG21	1.97	0.46
2:B:591:GLN:HA	2:B:594:LEU:HD12	1.98	0.46
1:A:9:GLU:OE2	1:A:16:MET:HG2	2.15	0.46
1:A:72:SER:OG	1:A:73:VAL:N	2.47	0.46
1:A:189:GLN:HG2	1:A:212:ASN:HA	1.97	0.46
1:A:917:HIS:CE1	1:A:919:SER:HB2	2.51	0.45
2:B:350:THR:OG1	2:B:373:ARG:HG3	2.16	0.45
2:B:347:LEU:HD22	2:B:373:ARG:HG2	1.99	0.45
1:A:195:TRP:CE3	1:A:204:LYS:HB2	2.51	0.45
1:A:282:MET:HA	1:A:283:PRO:HD2	1.82	0.45
1:A:969:GLN:H	1:A:969:GLN:CD	2.19	0.45
2:B:512:PHE:HB2	2:B:521:ILE:HD11	1.98	0.45
1:A:26:LEU:HD23	1:A:101:VAL:HG11	1.98	0.45
1:A:942:LYS:HD2	1:A:947:TYR:O	2.17	0.45
1:A:529:GLU:HA	1:A:532:LYS:HE2	1.97	0.45
1:A:833:MET:HE1	1:A:903:GLY:HA3	1.99	0.45
1:A:619:LEU:HD22	1:A:623:LEU:HD22	1.99	0.44
1:A:1044:ASN:ND2	1:A:1051:TRP:O	2.45	0.44
1:A:199:SER:HB2	1:A:200:PRO:HD2	1.99	0.44
1:A:934:PHE:O	1:A:936:HIS:N	2.50	0.44
1:A:46:LYS:HG2	1:A:65:GLU:HB3	1.99	0.44
1:A:1054:LYS:HA	1:A:1054:LYS:HD2	1.79	0.44
1:A:1024:LYS:HB2	1:A:1024:LYS:HE3	1.66	0.44
1:A:1053:THR:HB	1:A:1055:MET:H	1.83	0.44
2:B:371:THR:HA	2:B:379:LYS:O	2.17	0.44
1:A:121:ILE:HD11	1:A:692:CYS:SG	2.58	0.44
1:A:600:GLU:HB2	1:A:1000:ASN:ND2	2.33	0.44
1:A:489:MET:HA	1:A:492:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:947:TYR:CD1	1:A:949:ARG:HB3	2.53	0.43
1:A:148:LYS:HE2	1:A:148:LYS:HB3	1.59	0.43
1:A:1031:THR:HG22	1:A:1034:GLU:H	1.82	0.43
1:A:54:ARG:HA	1:A:59:HIS:CD2	2.52	0.43
1:A:121:ILE:CD1	1:A:688:LEU:HB3	2.48	0.43
1:A:521:ASN:HB2	1:A:557:TYR:OH	2.19	0.43
1:A:357:ARG:NH2	1:A:370:ASN:HD22	2.17	0.43
1:A:940:HIS:C	1:A:942:LYS:H	2.21	0.43
1:A:360:ILE:HG22	1:A:367:LEU:HD12	2.00	0.43
1:A:365:GLU:HG3	2:B:377:ASN:OD1	2.18	0.43
2:B:457:GLN:HA	2:B:460:SER:HB2	2.00	0.43
1:A:479:TRP:CZ3	1:A:481:SER:HA	2.53	0.43
2:B:412:SER:HA	2:B:423:LYS:HG2	2.01	0.42
1:A:917:HIS:HE1	1:A:919:SER:HB2	1.84	0.42
1:A:613:GLY:HA2	1:A:648:LEU:HD12	2.00	0.42
2:B:590:ARG:HB3	2:B:593:LYS:HG3	2.01	0.42
1:A:727:THR:HB	1:A:729:LYS:HD2	2.02	0.42
1:A:220:VAL:HB	1:A:252:LEU:HD11	2.02	0.42
1:A:180:HIS:ND1	1:A:828:GLY:HA2	2.35	0.42
1:A:297:LEU:HA	1:A:298:PRO:HD3	1.68	0.42
1:A:27:PRO:HG3	1:A:101:VAL:O	2.20	0.42
1:A:404:LEU:HD11	1:A:443:LEU:HD23	2.01	0.42
1:A:468:LYS:HD3	1:A:468:LYS:HA	1.93	0.42
1:A:216:VAL:O	1:A:219:GLN:HG2	2.20	0.41
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.88	0.41
1:A:776:LYS:HD2	1:A:804:GLY:HA3	2.03	0.41
2:B:382:LYS:HE3	2:B:382:LYS:HB2	1.92	0.41
1:A:532:LYS:O	1:A:536:THR:HG23	2.20	0.41
1:A:140:ARG:HD3	1:A:689:GLU:OE1	2.21	0.41
1:A:1048:HIS:C	1:A:1050:GLY:H	2.24	0.41
1:A:429:LEU:HA	1:A:429:LEU:HD23	1.83	0.41
2:B:583:TRP:CH2	2:B:587:LYS:HE2	2.56	0.41
2:B:354:THR:HA	2:B:426:TYR:O	2.21	0.41
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.95	0.41
1:A:676:HIS:CD2	1:A:843:ASP:HB2	2.56	0.41
1:A:181:ILE:HD12	1:A:278:MET:SD	2.61	0.40
1:A:223:GLU:O	1:A:226:ARG:HG2	2.21	0.40
2:B:593:LYS:O	2:B:596:GLU:HG2	2.21	0.40
1:A:357:ARG:HH21	1:A:370:ASN:HD22	1.70	0.40
1:A:187:LYS:HE3	1:A:187:LYS:HB2	1.83	0.40
1:A:42:LEU:HD11	1:A:82:PHE:HB3	2.03	0.40
1:A:904:TYR:CE1	1:A:930:PHE:HA	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:GLU:HB2	1:A:88:ARG:HE	1.86	0.40
1:A:834:LEU:HD12	1:A:834:LEU:HA	1.82	0.40
1:A:178:PRO:HB2	1:A:181:ILE:HG12	2.04	0.40
1:A:151:VAL:HG12	1:A:154:ARG:NH2	2.37	0.40
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.57	0.40
1:A:857:ILE:HA	1:A:857:ILE:HD13	1.90	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	982/1068 (92%)	932 (95%)	48 (5%)	2 (0%)	56 81
2	B	275/324 (85%)	266 (97%)	8 (3%)	1 (0%)	43 70
All	All	1257/1392 (90%)	1198 (95%)	56 (4%)	3 (0%)	56 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	935	GLY
2	B	515	GLU
1	A	264	LYS

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	910/974 (93%)	864 (95%)	46 (5%)	33 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	258/301 (86%)	242 (94%)	16 (6%)	26 48
All	All	1168/1275 (92%)	1106 (95%)	62 (5%)	32 57

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	60	GLN
1	A	89	LEU
1	A	93	ARG
1	A	101	VAL
1	A	109	GLU
1	A	115	ARG
1	A	121	ILE
1	A	140	ARG
1	A	162	ARG
1	A	187	LYS
1	A	197	ILE
1	A	219	GLN
1	A	223	GLU
1	A	225	ILE
1	A	281	ARG
1	A	292	SER
1	A	301	CYS
1	A	329	VAL
1	A	358	THR
1	A	369	ASP
1	A	378	CYS
1	A	475	LEU
1	A	488	ASP
1	A	490	SER
1	A	576	SER
1	A	626	ASP
1	A	681	SER
1	A	682	GLN
1	A	687	LEU
1	A	700	LYS
1	A	729	LYS
1	A	774	SER
1	A	784	GLU
1	A	788	ILE
1	A	862	CYS

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Mol	Chain	Res	Type
1	A	875	HIS
1	A	883	ASP
1	A	901	CYS
1	A	942	LYS
1	A	945	PHE
1	A	947	TYR
1	A	959	ASP
1	A	974	THR
1	A	1031	THR
1	A	1053	THR
2	B	325	ASN
2	B	419	LYS
2	B	433	GLN
2	B	440	ASP
2	B	454	THR
2	B	455	GLN
2	B	460	SER
2	B	487	PHE
2	B	501	GLN
2	B	509	ILE
2	B	524	ILE
2	B	525	MET
2	B	536	SER
2	B	542	ARG
2	B	548	ASP
2	B	581	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	60	GLN
1	A	201	ASN
1	A	370	ASN
1	A	444	ASN
1	A	795	GLN

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 ⓘ

1 ligand is 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	SO4	B	701	-	4,4,4	0.16	0	6,6,6	0.07	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	SO4	B	701	-	-	0/0/0/0	0/0/0/0

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.

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	994/1068 (93%)	0.56	67 (6%)	17 16	38, 63, 109, 164	0
2	B	277/324 (85%)	0.54	24 (8%)	10 8	45, 70, 123, 135	0
All	All	1271/1392 (91%)	0.56	91 (7%)	15 13	38, 65, 114, 164	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	8.1
1	A	947	TYR	5.4
1	A	202	ASN	5.4
1	A	243	VAL	5.3
1	A	197	ILE	5.0
1	A	221	ILE	4.7
1	A	1055	MET	4.5
1	A	945	PHE	4.4
2	B	507	GLU	4.4
2	B	509	ILE	4.2
1	A	298	PRO	4.2
2	B	508	TYR	4.0
1	A	70	PHE	3.8
1	A	481	SER	3.8
2	B	597	TRP	3.8
1	A	207	TYR	3.6
2	B	438	LYS	3.6
2	B	513	LYS	3.5
1	A	156	LEU	3.4
1	A	323	SER	3.4
2	B	598	LEU	3.2
1	A	1057	TRP	3.2
2	B	435	GLN	3.2
2	B	442	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	510	GLU	3.1
2	B	511	LYS	3.1
1	A	414	GLY	3.0
1	A	194	ILE	3.0
1	A	196	VAL	3.0
2	B	439	GLU	3.0
1	A	944	LYS	3.0
1	A	220	VAL	2.8
1	A	61	LEU	2.8
1	A	246	TYR	2.8
1	A	1054	LYS	2.7
1	A	295	SER	2.7
1	A	293	LEU	2.7
1	A	86	THR	2.7
1	A	186	ASP	2.6
1	A	211	ILE	2.6
1	A	306	SER	2.5
1	A	297	LEU	2.5
1	A	792	LEU	2.5
1	A	69	ILE	2.5
1	A	62	LEU	2.5
1	A	267	LEU	2.5
1	A	744	PHE	2.5
2	B	583	TRP	2.5
1	A	307	TYR	2.5
1	A	200	PRO	2.4
1	A	250	TYR	2.4
1	A	191	ILE	2.4
2	B	504	TYR	2.4
1	A	205	GLN	2.4
2	B	506	LYS	2.4
1	A	1058	ILE	2.4
1	A	245	GLU	2.4
1	A	499	SER	2.4
1	A	500	VAL	2.3
1	A	722	GLU	2.3
1	A	943	LYS	2.3
1	A	285	LEU	2.3
1	A	881	LEU	2.3
2	B	457	GLN	2.3
1	A	43	ILE	2.3
2	B	538	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	522	GLU	2.3
2	B	501	GLN	2.2
1	A	209	LEU	2.2
1	A	793	LEU	2.2
2	B	514	ARG	2.2
1	A	13	ILE	2.2
2	B	589	VAL	2.2
1	A	294	TYR	2.2
1	A	633	ILE	2.2
1	A	1046	ALA	2.2
1	A	875	HIS	2.2
1	A	198	VAL	2.1
1	A	10	LEU	2.1
1	A	15	LEU	2.1
1	A	68	TYR	2.1
2	B	322	MET	2.1
1	A	82	PHE	2.1
1	A	99	LEU	2.1
2	B	516	GLY	2.1
1	A	180	HIS	2.1
1	A	224	ALA	2.1
1	A	671	LEU	2.1
2	B	523	ARG	2.1
1	A	226	ARG	2.0
2	B	434	ASP	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(\AA^2)	Q<0.9
3	SO4	B	701	5/5	0.12	-0.79	63,66,68,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.