Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 06:16 AM EDT

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 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 (i) 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 (i)) were used in the production of this report:

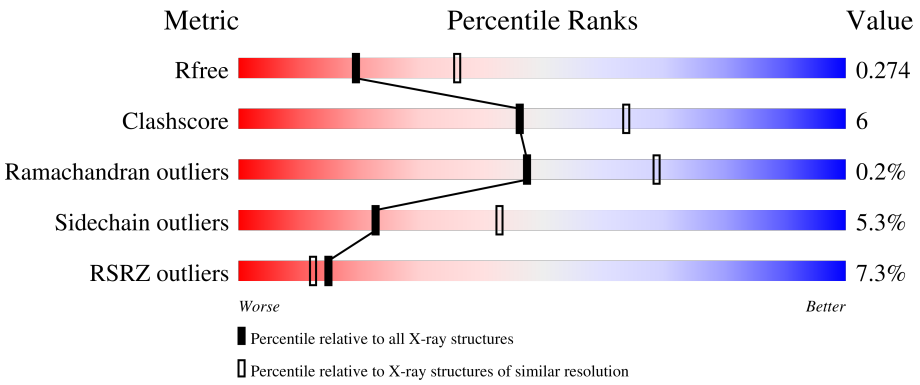
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (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 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 <=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	7% 75% 17% • 7%
2	B	324	7% 67% 16% • 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10528 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
			Total	C	N	O	S			
1	A	994	8132	5205	1383	1476	68	0	0	0

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

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

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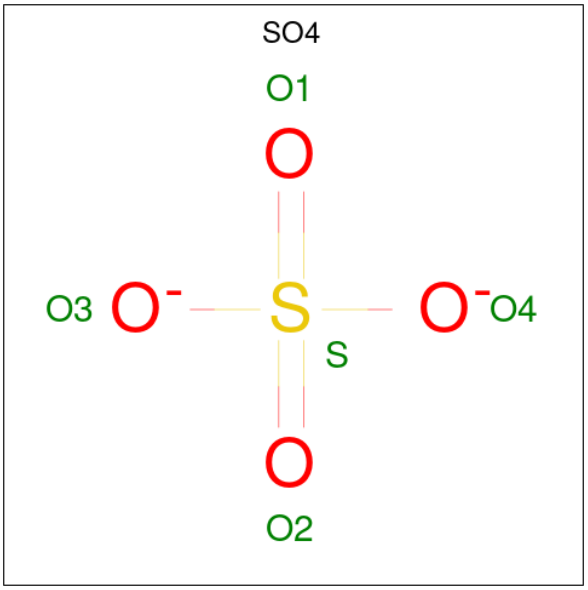
Chain	Residue	Modelled	Actual	Comment	Reference
B	311	LEU	-	expression tag	UNP P27986
B	312	TYR	-	expression tag	UNP P27986
B	313	PHE	-	expression tag	UNP P27986
B	314	GLN	-	expression tag	UNP P27986
B	315	SER	-	expression tag	UNP P27986
B	316	ILE	-	expression tag	UNP P27986
B	317	ALA	-	expression tag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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

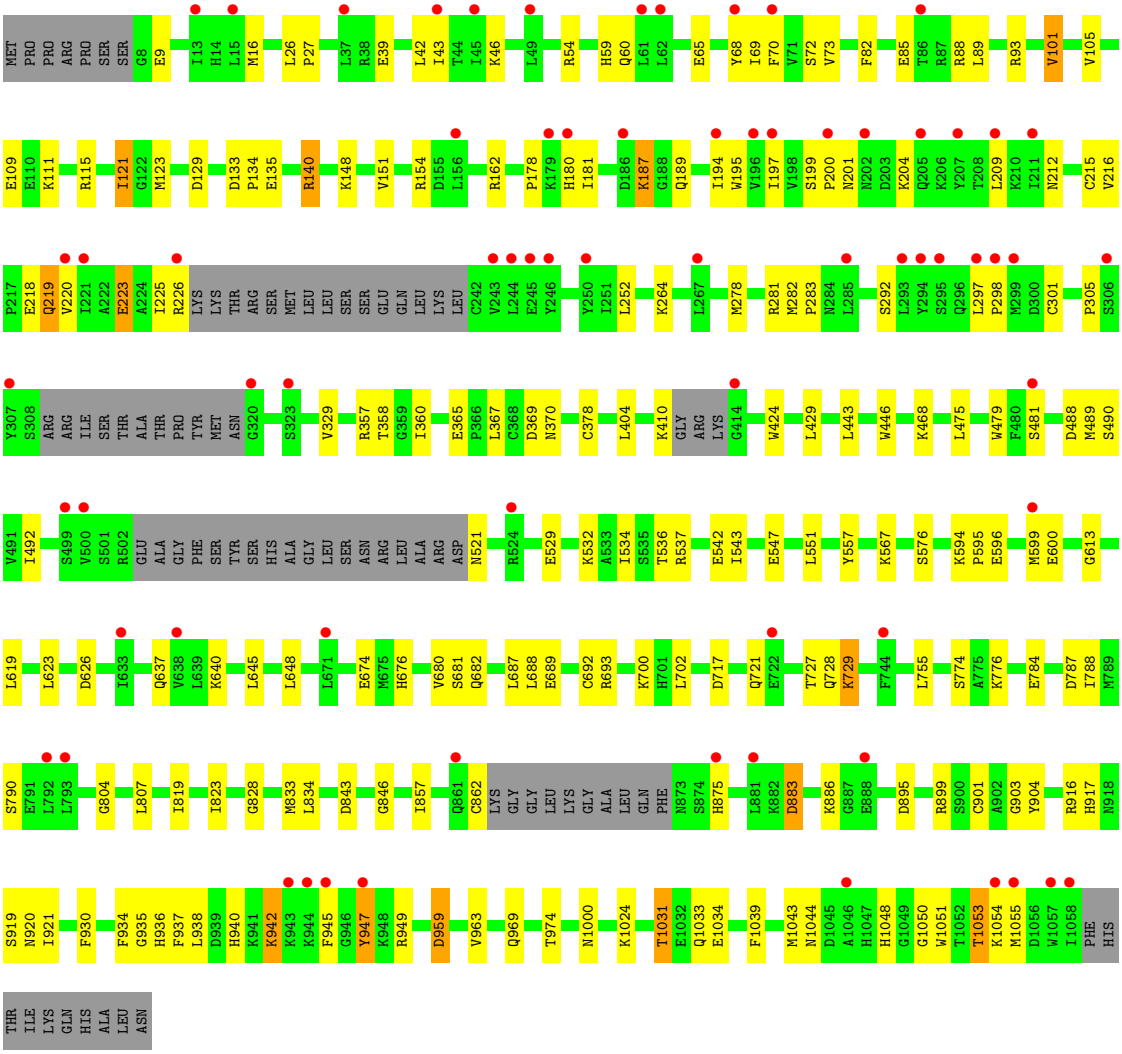
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	31	31	31	0	0
			Total	O		
4	B	6	6	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

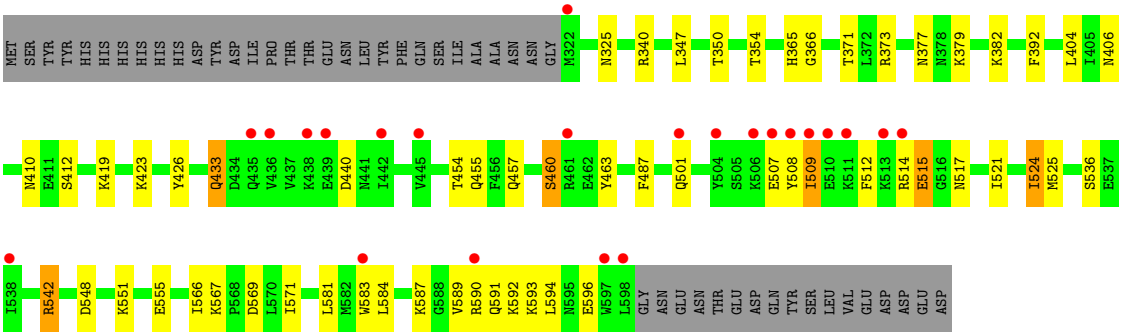
• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

Chain A: 7% 75% 17% • 7%



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B: 7% 67% 16% • 15%


MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN SER ILE ALA ALA ASN ASN GLY
M322 N325 R340 L347 T350 T354 H365 G366 T371 L372 R373 N377 N378 K379 K382 F392 L404 I405 N406
N410 E411 S412 K419 K423 Y426 Q433 D434 Q435 V436 V437 K438 E439 D440 N441 I442 V445 T454 Q455 F456 Q457 S460 R461 E462 Y463 F487 Q501 Y504 S505 K506 E507 Y508 I509 E510 K511 F512 K513 R514 E515 G516 N517 I521 I524 M525 S536 E537
I538 R542 D548 K551 E555 I566 K567 P568 D569 L570 I571 L581 M582 W583 L584 K587 G588 V589 R590 Q591 K592 K593 L594 N595 E596 W597 L598 GLY ASN GLU ASN THR GLU ASP GLN TYR SER LEU VAL GLU ASP ASP GLU ASP

4 Data and refinement statistics (i)

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) 95.4 (47.09-2.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.217 , 0.274 0.217 , 0.274	Depositor DCC
R_{free} test set	2329 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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 Too-close contacts (i)

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	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

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 6.

All (132) 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: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
1:A:937:PHE:HD1	1:A:938:LEU:HG	1.69	0.56
2:B:507:GLU:HG3	2:B:508:TYR:HD1	1.70	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:HG2	2:B:542:ARG:NH1	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	Interatomic distance (Å)	Clash overlap (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:819:ILE:O	1:A:823:ILE:HG12	2.13	0.47
1:A:883:ASP:HA	1:A:886:LYS:HD3	1.96	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:542:GLU:OE1	2:B:340:ARG:HD3	2.15	0.47
1:A:728:GLN:HB2	1:A:729:LYS:HE3	1.97	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:347:LEU:HD22	2:B:373:ARG:HG2	1.99	0.45
2:B:350:THR:OG1	2:B:373:ARG:HG3	2.16	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:529:GLU:HA	1:A:532:LYS:HE2	1.97	0.45
1:A:942:LYS:HD2	1:A:947:TYR:O	2.17	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:46:LYS:HG2	1:A:65:GLU:HB3	1.99	0.44
1:A:934:PHE:O	1:A:936:HIS:N	2.50	0.44
1:A:1054:LYS:HA	1:A:1054:LYS:HD2	1.79	0.44
1:A:1024:LYS:HE3	1:A:1024:LYS:HB2	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:489:MET:HA	1:A:492:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:GLU:HB2	1:A:1000:ASN:ND2	2.33	0.44
1:A:148:LYS:HE2	1:A:148:LYS:HB3	1.59	0.43
1:A:947:TYR:CD1	1:A:949:ARG:HB3	2.53	0.43
1:A:54:ARG:HA	1:A:59:HIS:CD2	2.52	0.43
1:A:1031:THR:HG22	1:A:1034:GLU:H	1.82	0.43
1:A:121:ILE:CD1	1:A:688:LEU:HB3	2.48	0.43
1:A:357:ARG:NH2	1:A:370:ASN:HD22	2.17	0.43
1:A:521:ASN:HB2	1:A:557:TYR:OH	2.19	0.43
1:A:360:ILE:HG22	1:A:367:LEU:HD12	2.00	0.43
1:A:940:HIS:C	1:A:942:LYS:H	2.21	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:613:GLY:HA2	1:A:648:LEU:HD12	2.00	0.42
1:A:917:HIS:HE1	1:A:919:SER:HB2	1.84	0.42
1:A:727:THR:HB	1:A:729:LYS:HD2	2.02	0.42
2:B:590:ARG:HB3	2:B:593:LYS:HG3	2.01	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:HA	1:A:468:LYS:HD3	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:429:LEU:HD23	1:A:429:LEU:HA	1.83	0.41
1:A:1048:HIS:C	1:A:1050:GLY:H	2.24	0.41
1:A:676:HIS:CD2	1:A:843:ASP:HB2	2.56	0.41
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.95	0.41
2:B:354:THR:HA	2:B:426:TYR:O	2.21	0.41
2:B:583:TRP:CH2	2:B:587:LYS:HE2	2.56	0.41
1:A:181:ILE:HD12	1:A:278:MET:SD	2.61	0.40
1:A:187:LYS:HB2	1:A:187:LYS:HE3	1.83	0.40
1:A:223:GLU:O	1:A:226:ARG:HG2	2.21	0.40
1:A:357:ARG:HH21	1:A:370:ASN:HD22	1.70	0.40
2:B:593:LYS:O	2:B:596:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HB2	1:A:88:ARG:HE	1.86	0.40
1:A:42:LEU:HD11	1:A:82:PHE:HB3	2.03	0.40
1:A:834:LEU:HD12	1:A:834:LEU:HA	1.82	0.40
1:A:904:TYR:CE1	1:A:930:PHE:HA	2.56	0.40
1:A:151:VAL:HG12	1:A:154:ARG:NH2	2.37	0.40
1:A:178:PRO:HB2	1:A:181:ILE:HG12	2.04	0.40
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.57	0.40
1:A:857:ILE:HD13	1:A:857:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	982/1068 (92%)	932 (95%)	48 (5%)	2 (0%)	47	69
2	B	275/324 (85%)	266 (97%)	8 (3%)	1 (0%)	34	55
All	All	1257/1392 (90%)	1198 (95%)	56 (4%)	3 (0%)	47	69

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	910/974 (93%)	864 (95%)	46 (5%)	24	44
2	B	258/301 (86%)	242 (94%)	16 (6%)	18	35
All	All	1168/1275 (92%)	1106 (95%)	62 (5%)	22	43

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

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Mol	Chain	Res	Type
1	A	784	GLU
1	A	788	ILE
1	A	862	CYS
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

Sometimes 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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	0.15	0	6,6,6	0.10	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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.55	70 (7%)	16	13	38, 63, 109, 164	0
2	B	277/324 (85%)	0.49	23 (8%)	11	9	45, 70, 123, 135	0
All	All	1271/1392 (91%)	0.54	93 (7%)	15	12	38, 65, 114, 164	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	7.9
1	A	243	VAL	6.1
1	A	202	ASN	6.0
1	A	197	ILE	4.9
1	A	1055	MET	4.8
1	A	947	TYR	4.7
1	A	156	LEU	4.7
1	A	298	PRO	4.5
2	B	507	GLU	4.4
1	A	221	ILE	4.2
1	A	945	PHE	4.0
1	A	1057	TRP	3.9
2	B	509	ILE	3.9
1	A	481	SER	3.8
2	B	435	GLN	3.8
1	A	70	PHE	3.8
2	B	508	TYR	3.6
1	A	414	GLY	3.5
1	A	323	SER	3.4
2	B	438	LYS	3.4
2	B	510	GLU	3.2
1	A	295	SER	3.1
1	A	793	LEU	3.1
2	B	598	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	442	ILE	3.0
1	A	1054	LYS	3.0
1	A	186	ASP	2.9
1	A	207	TYR	2.9
1	A	297	LEU	2.9
1	A	944	LYS	2.9
1	A	792	LEU	2.9
1	A	13	ILE	2.8
1	A	62	LEU	2.8
2	B	322	MET	2.8
2	B	513	LYS	2.8
1	A	220	VAL	2.7
1	A	293	LEU	2.7
1	A	285	LEU	2.7
2	B	597	TRP	2.7
1	A	1046	ALA	2.7
2	B	436	VAL	2.6
1	A	671	LEU	2.6
1	A	61	LEU	2.6
1	A	245	GLU	2.6
2	B	511	LYS	2.6
1	A	86	THR	2.5
1	A	200	PRO	2.5
1	A	722	GLU	2.5
1	A	1058	ILE	2.4
1	A	209	LEU	2.4
1	A	194	ILE	2.4
2	B	583	TRP	2.4
1	A	49	LEU	2.4
2	B	439	GLU	2.3
1	A	226	ARG	2.3
1	A	267	LEU	2.3
2	B	590	ARG	2.3
1	A	211	ILE	2.3
1	A	250	TYR	2.3
1	A	500	VAL	2.3
2	B	445	VAL	2.3
1	A	299	MET	2.3
1	A	306	SER	2.3
1	A	744	PHE	2.3
1	A	633	ILE	2.3
1	A	37	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	506	LYS	2.2
1	A	205	GLN	2.2
1	A	881	LEU	2.2
1	A	68	TYR	2.2
1	A	246	TYR	2.2
1	A	43	ILE	2.2
1	A	45	ILE	2.1
1	A	499	SER	2.1
2	B	501	GLN	2.1
2	B	514	ARG	2.1
1	A	888	GLU	2.1
1	A	196	VAL	2.1
2	B	504	TYR	2.1
1	A	524	ARG	2.1
1	A	180	HIS	2.1
1	A	861	GLN	2.1
1	A	15	LEU	2.1
1	A	875	HIS	2.1
1	A	599	MET	2.1
2	B	461	ARG	2.1
1	A	307	TYR	2.1
1	A	320	GLY	2.1
1	A	294	TYR	2.0
1	A	943	LYS	2.0
2	B	538	ILE	2.0
1	A	179	LYS	2.0
1	A	638	VAL	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 monosaccharides 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(Å^2)	Q<0.9
3	SO4	B	701	5/5	0.97	0.13	63,66,68,70	0

6.5 Other polymers (i)

There are no such residues in this entry.