



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:12 AM GMT

PDB ID : 4L2Y
Title : Crystal Structure of p110alpha complexed with niSH2 of p85alpha and compound 9d
Authors : Zhang, J.; Zhao, Y.L.; Chen, Y.Y.; Huang, M.; Jiang, F.
Deposited on : 2013-06-05
Resolution : 2.80 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>

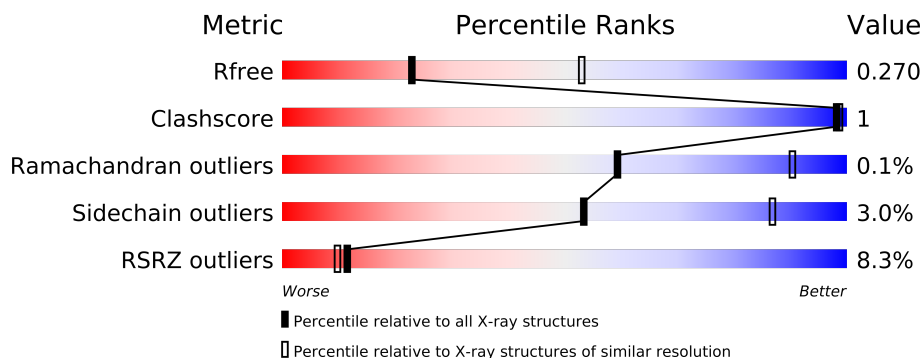
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 10533 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	991	Total	C	N	O	S	0	0	0
			8119	5198	1384	1470	67			

- 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:

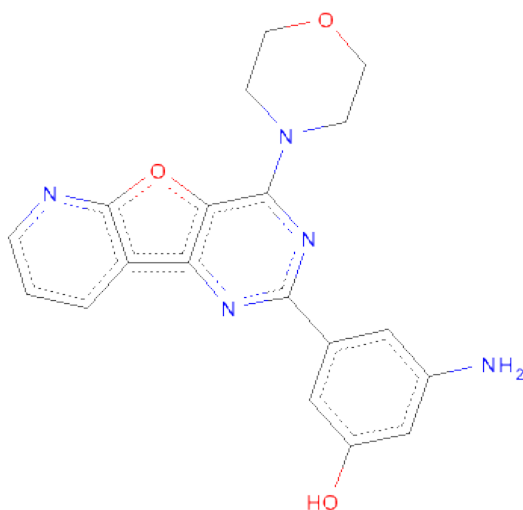
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	MET	-	EXPRESSION TAG	UNP P27986
B	293	SER	-	EXPRESSION TAG	UNP P27986
B	294	TYR	-	EXPRESSION TAG	UNP P27986
B	295	TYR	-	EXPRESSION TAG	UNP P27986
B	296	HIS	-	EXPRESSION TAG	UNP P27986
B	297	HIS	-	EXPRESSION TAG	UNP P27986
B	298	HIS	-	EXPRESSION TAG	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-AMINO-5-[4-(MORPHOLIN-4-YL)PYRIDO[3',2':4,5]FURO[3,2-D]PYRIMIDIN-2-YL]PHENOL (three-letter code: XXK) (formula: C₁₉H₁₇N₅O₃).



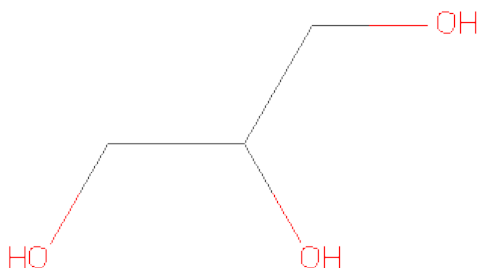
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	5	3		

- 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	A	1	Total	C	O	0	0
			6	3	3		

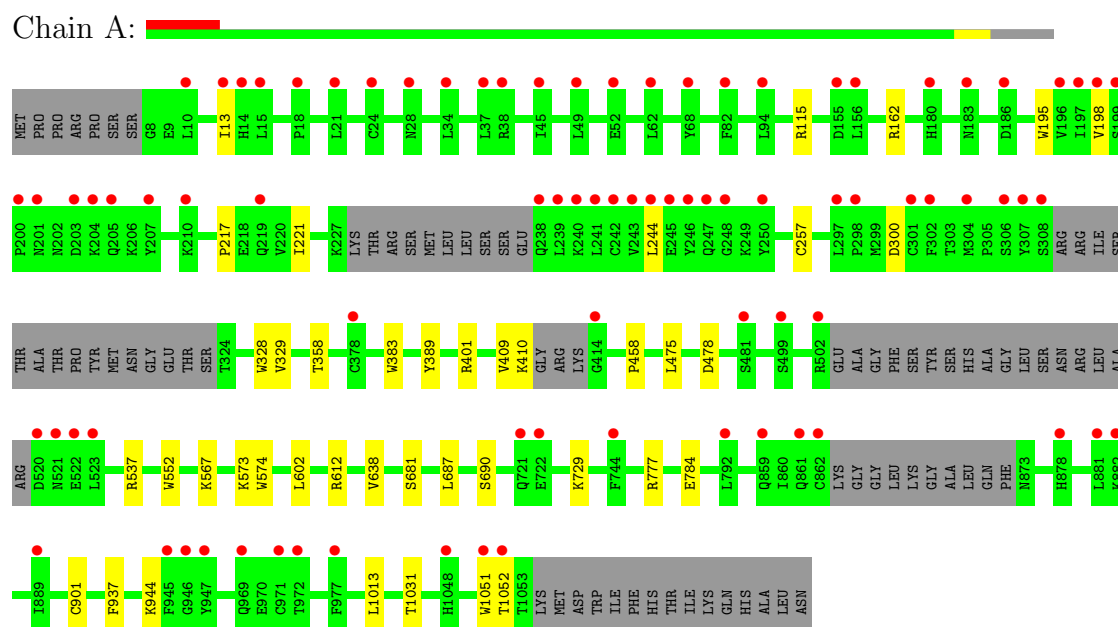
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		

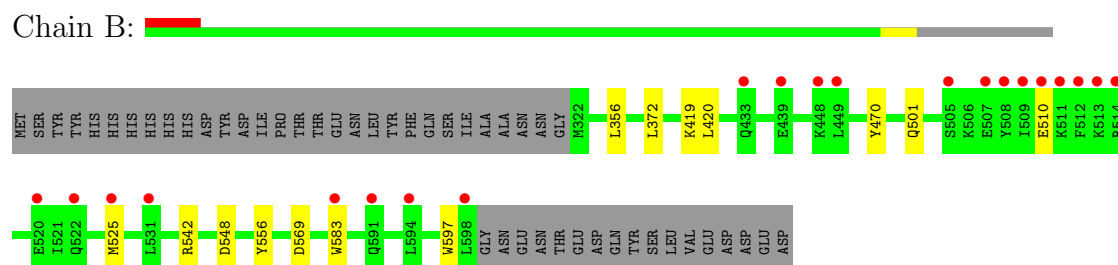
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.94Å 136.97Å 150.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.80 48.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.30-2.80) 96.3 (48.30-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.215 , 0.271 0.215 , 0.270	Depositor DCC
R_{free} test set	1781 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 35584 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10533	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: XXK, GOL, 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	0.46	6/8301 (0.1%)	0.50	0/11219
2	B	0.42	2/2394 (0.1%)	0.49	0/3207
All	All	0.45	8/10695 (0.1%)	0.50	0/14426

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	TRP	CD2-CE2	5.25	1.47	1.41
1	A	552	TRP	CD2-CE2	5.25	1.47	1.41
1	A	1051	TRP	CD2-CE2	5.16	1.47	1.41
1	A	574	TRP	CD2-CE2	5.11	1.47	1.41
1	A	383	TRP	CD2-CE2	5.06	1.47	1.41
1	A	195	TRP	CD2-CE2	5.05	1.47	1.41
2	B	583	TRP	CD2-CE2	5.04	1.47	1.41
2	B	597	TRP	CD2-CE2	5.04	1.47	1.41

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	8119	0	0	5	0
2	B	2354	0	0	2	0
3	A	27	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	6	0	8	0	0
6	A	17	0	0	0	0
All	All	10533	0	8	6	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 1.

All (6) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:410:LYS:NZ	2:B:569:ASP:OD1	2.39	0.55
1:A:537:ARG:O	1:A:567:LYS:NZ	2.43	0.51
1:A:401:ARG:NH2	1:A:458:PRO:O	2.44	0.50
1:A:358:THR:CG2	1:A:389:TYR:OH	2.65	0.45
2:B:470:TYR:OH	2:B:556:TYR:OH	2.35	0.44
1:A:602:LEU:O	1:A:612:ARG:NH2	2.53	0.41

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	979/1068 (92%)	942 (96%)	36 (4%)	1 (0%)	59	90
2	B	275/324 (85%)	272 (99%)	3 (1%)	0	100	100
All	All	1254/1392 (90%)	1214 (97%)	39 (3%)	1 (0%)	59	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	PRO

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%)	884 (97%)	26 (3%)	55	88
2	B	258/301 (86%)	249 (96%)	9 (4%)	48	83
All	All	1168/1275 (92%)	1133 (97%)	35 (3%)	53	87

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	115	ARG
1	A	162	ARG
1	A	198	VAL
1	A	221	ILE
1	A	244	LEU
1	A	257	CYS
1	A	300	ASP
1	A	329	VAL
1	A	409	VAL
1	A	475	LEU
1	A	478	ASP
1	A	573	LYS
1	A	638	VAL
1	A	681	SER
1	A	687	LEU
1	A	690	SER
1	A	729	LYS
1	A	777	ARG
1	A	784	GLU
1	A	901	CYS
1	A	937	PHE
1	A	944	LYS
1	A	1013	LEU
1	A	1031	THR
1	A	1052	THR
2	B	356	LEU
2	B	372	LEU
2	B	419	LYS

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Mol	Chain	Res	Type
2	B	420	LEU
2	B	501	GLN
2	B	510	GLU
2	B	525	MET
2	B	542	ARG
2	B	548	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	XXK	A	1101	-	29,31,31	1.29	4 (13%)	37,45,45	2.09	10 (27%)
4	SO4	A	1102	-	4,4,4	0.42	0	6,6,6	0.07	0
5	GOL	A	1103	-	5,5,5	0.23	0	5,5,5	0.25	0
4	SO4	B	701	-	4,4,4	0.36	0	6,6,6	0.13	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	XXK	A	1101	-	-	0/8/16/16	0/2/5/5
4	SO4	A	1102	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1103	-	-	0/4/4/4	0/0/0/0
4	SO4	B	701	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	XXK	C22-N28	2.91	1.49	1.38
3	A	1101	XXK	C19-N10	2.88	1.37	1.32
3	A	1101	XXK	C05-C09	2.63	1.46	1.41
3	A	1101	XXK	C11-N18	2.30	1.36	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	XXK	C13-N12-C17	6.30	124.64	111.67
3	A	1101	XXK	C11-N18-C19	4.87	124.30	116.16
3	A	1101	XXK	N10-C19-N18	-4.40	123.17	126.10
3	A	1101	XXK	C05-C06-N01	-3.36	119.09	124.93
3	A	1101	XXK	C05-C09-C08	-3.28	104.34	108.49
3	A	1101	XXK	C03-C04-C05	-3.25	114.98	120.74
3	A	1101	XXK	N18-C11-N12	2.99	120.05	116.97
3	A	1101	XXK	O07-C08-C09	2.52	111.64	107.42
3	A	1101	XXK	C08-C11-N18	-2.29	115.35	120.67
3	A	1101	XXK	C04-C05-C06	2.28	122.85	118.70

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	991/1068 (92%)	0.56	85 (8%) 11 9	43, 77, 134, 206	2 (0%)
2	B	277/324 (85%)	0.43	21 (7%) 14 12	54, 81, 139, 171	0
All	All	1268/1392 (91%)	0.53	106 (8%) 11 9	43, 79, 135, 206	2 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	862	CYS	11.7
1	A	238	GLN	7.9
1	A	239	LEU	5.6
1	A	246	TYR	5.3
1	A	240	LYS	5.1
2	B	520	GLU	5.0
2	B	514	ARG	4.9
1	A	197	ILE	4.9
1	A	248	GLY	4.9
1	A	200	PRO	4.9
1	A	241	LEU	4.8
1	A	62	LEU	4.7
2	B	509	ILE	4.6
1	A	244	LEU	4.6
1	A	1052	THR	4.5
2	B	508	TYR	4.5
1	A	207	TYR	4.4
1	A	196	VAL	4.4
1	A	155	ASP	4.4
1	A	201	ASN	4.4
1	A	242	CYS	4.2
1	A	82	PHE	4.2
1	A	972	THR	4.1
1	A	946	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	439	GLU	4.0
1	A	1048	HIS	3.9
1	A	301	CYS	3.9
1	A	243	VAL	3.9
1	A	247	GLN	3.8
1	A	10	LEU	3.8
1	A	414	GLY	3.6
1	A	481	SER	3.6
2	B	511	LYS	3.5
1	A	156	LEU	3.5
1	A	520	ASP	3.5
1	A	14	HIS	3.4
1	A	304	MET	3.4
1	A	203	ASP	3.4
1	A	306	SER	3.3
1	A	15	LEU	3.3
2	B	507	GLU	3.2
1	A	861	GLN	3.2
2	B	513	LYS	3.1
1	A	969	GLN	3.1
2	B	510	GLU	3.1
1	A	186	ASP	3.1
1	A	37	LEU	3.0
1	A	45	ILE	3.0
1	A	308	SER	2.9
1	A	521	ASN	2.9
1	A	302	PHE	2.9
1	A	52	GLU	2.8
2	B	583	TRP	2.8
1	A	94	LEU	2.8
1	A	307	TYR	2.7
1	A	1051	TRP	2.7
2	B	525	MET	2.7
1	A	38	ARG	2.7
1	A	199	SER	2.7
1	A	68	TYR	2.7
2	B	448	LYS	2.7
2	B	522	GLN	2.7
2	B	598	LEU	2.6
1	A	18	PRO	2.6
1	A	245	GLU	2.6
1	A	522	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	859	GLN	2.6
2	B	591	GLN	2.6
1	A	219	GLN	2.5
1	A	21	LEU	2.5
1	A	180	HIS	2.5
1	A	298	PRO	2.5
1	A	721	GLN	2.5
1	A	250	TYR	2.5
1	A	378	CYS	2.5
2	B	505	SER	2.5
1	A	722	GLU	2.4
1	A	744	PHE	2.4
2	B	433	GLN	2.3
1	A	297	LEU	2.3
1	A	204	LYS	2.3
1	A	523	LEU	2.3
1	A	792	LEU	2.3
1	A	881	LEU	2.3
2	B	449	LEU	2.3
1	A	198	VAL	2.3
1	A	183	ASN	2.2
2	B	512	PHE	2.2
1	A	210	LYS	2.2
1	A	49	LEU	2.2
1	A	971	CYS	2.2
1	A	878	HIS	2.1
1	A	205	GLN	2.1
1	A	947	TYR	2.1
1	A	13	ILE	2.1
1	A	28	ASN	2.1
1	A	502	ARG	2.1
1	A	945	PHE	2.1
1	A	34	LEU	2.1
2	B	594	LEU	2.1
1	A	24	CYS	2.1
2	B	531	LEU	2.1
1	A	889	ILE	2.0
1	A	499	SER	2.0
1	A	977	PHE	2.0
1	A	882	LYS	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
5	GOL	A	1103	6/6	0.24	1.95	69,72,72,75	0
4	SO4	B	701	5/5	0.19	1.00	79,79,79,82	0
4	SO4	A	1102	5/5	0.23	0.63	125,127,130,131	0
3	XXK	A	1101	27/27	0.20	-0.13	54,57,62,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.