



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:34 PM GMT

PDB ID : 3O2F
Title : Structure of the N-domain of GRP94 bound to the HSP90 inhibitor PU-H54
Authors : Seidler, P.M.; Gewirth, D.T.
Deposited on : 2010-07-22
Resolution : 2.00 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>

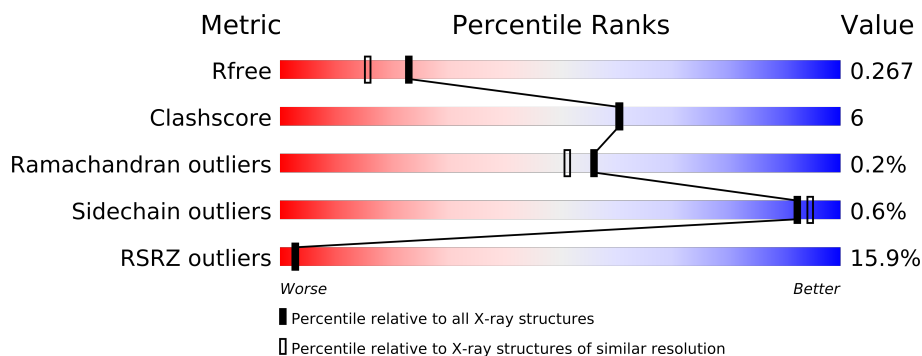
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	236	
1	B	236	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	3	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3703 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.

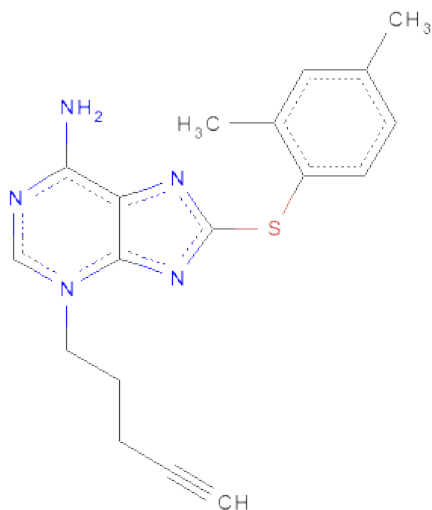
- Molecule 1 is a protein called Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1768	1122	291	350	5			
1	B	218	Total	C	N	O	S	0	0	0
			1649	1043	276	325	5			

There are 16 discrepancies between the modelled and reference sequences:

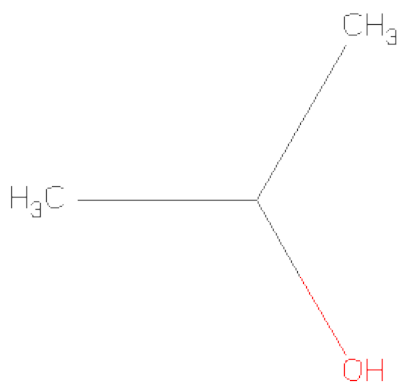
Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	EXPRESSION TAG	UNP P41148
A	66	SER	-	EXPRESSION TAG	UNP P41148
A	67	HIS	-	EXPRESSION TAG	UNP P41148
A	68	MET	-	EXPRESSION TAG	UNP P41148
A	287	GLY	-	LINKER	UNP P41148
A	288	GLY	-	LINKER	UNP P41148
A	289	GLY	-	LINKER	UNP P41148
A	290	GLY	-	LINKER	UNP P41148
B	65	GLY	-	EXPRESSION TAG	UNP P41148
B	66	SER	-	EXPRESSION TAG	UNP P41148
B	67	HIS	-	EXPRESSION TAG	UNP P41148
B	68	MET	-	EXPRESSION TAG	UNP P41148
B	287	GLY	-	LINKER	UNP P41148
B	288	GLY	-	LINKER	UNP P41148
B	289	GLY	-	LINKER	UNP P41148
B	290	GLY	-	LINKER	UNP P41148

- Molecule 2 is 8-[(2,4-DIMETHYLPHENYL)SULFANYL]-3-PENT-4-YN-1-YL-3H-PURIN-6-AMINE (three-letter code: P54) (formula: C₁₈H₁₉N₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			24	18	5	1		
2	B	1	Total	C	N	S	0	0
			24	18	5	1		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



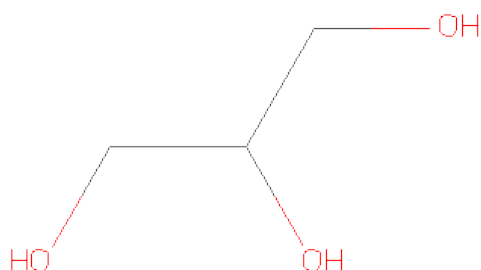
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

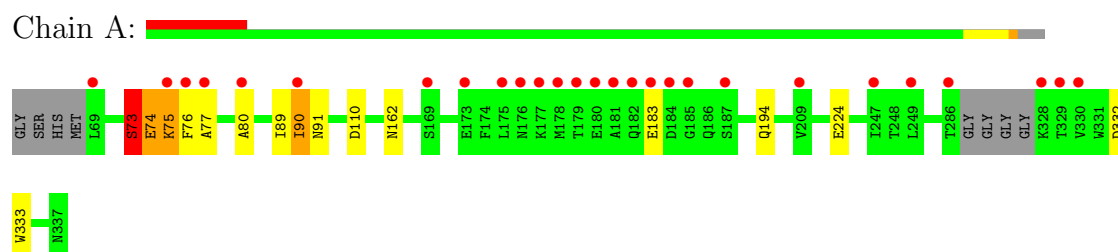
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	64	Total	O	0	0
			64	64		

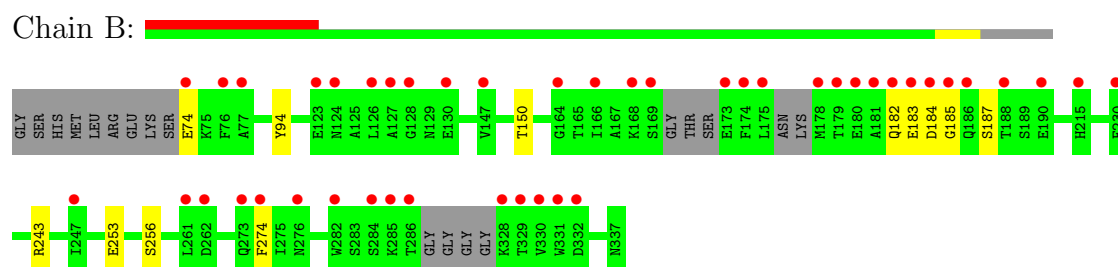
3 Residue-property plots

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: Endoplasmin



- Molecule 1: Endoplasmin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.96Å 65.69Å 85.45Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	32.84 – 2.00 32.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.84-2.00) 99.6 (32.54-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.269 0.236 , 0.267	Depositor DCC
R_{free} test set	2251 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	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	2 of 45178 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3703	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.62% 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: P54, GOL, IPA

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	0.67	0/1794	0.70	0/2425
1	B	0.45	0/1670	0.56	0/2263
All	All	0.57	0/3464	0.63	0/4688

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLU	Peptide
1	A	73	SER	Peptide
1	A	74	GLU	Peptide
1	A	75	LYS	Peptide
1	B	182	GLN	Peptide
1	B	183	GLU	Peptide
1	B	185	GLY	Peptide

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	1768	0	0	14	0
1	B	1649	0	0	7	0
2	A	24	0	19	0	0
2	B	24	0	17	0	0
3	A	16	0	32	4	0
4	A	6	0	8	0	0
5	A	152	0	0	1	0
5	B	64	0	0	1	0
All	All	3703	0	76	21	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 (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:184:ASP:O	1:B:187:SER:CB	2.30	0.79
1:B:184:ASP:O	1:B:187:SER:N	2.30	0.65
1:A:162:ASN:ND2	5:A:366:HOH:O	2.32	0.61
1:A:224:GLU:OE1	3:A:4:IPA:H12	2.02	0.59
1:A:91:ASN:OD1	1:A:91:ASN:C	2.42	0.58
1:A:90:ILE:O	1:A:90:ILE:CG2	2.52	0.57
1:A:332:ASP:OD1	1:A:333:TRP:N	2.37	0.57
1:B:74:GLU:N	5:B:383:HOH:O	2.38	0.56
1:B:184:ASP:O	1:B:187:SER:CA	2.53	0.56
1:A:75:LYS:N	1:A:76:PHE:CD2	2.77	0.51
1:A:224:GLU:OE2	3:A:4:IPA:H33	2.10	0.51
1:A:110:ASP:OD2	1:A:194:GLN:NE2	2.45	0.50
1:A:77:ALA:O	1:A:80:ALA:CB	2.60	0.50
1:A:91:ASN:OD1	1:A:91:ASN:O	2.32	0.47
1:B:253:GLU:O	1:B:256:SER:OG	2.31	0.47
1:A:89:ILE:C	1:A:91:ASN:N	2.69	0.46
3:A:2:IPA:H12	1:B:94:TYR:CE2	2.52	0.45
1:A:73:SER:CB	1:A:76:PHE:CZ	3.00	0.45
1:B:150:THR:O	1:B:243:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:GLU:CG	1:A:75:LYS:CA	2.97	0.43
1:A:89:ILE:CG2	3:A:2:IPA:H2	2.49	0.43

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	224/236 (95%)	211 (94%)	12 (5%)	1 (0%)	43	36
1	B	210/236 (89%)	200 (95%)	10 (5%)	0	100	100
All	All	434/472 (92%)	411 (95%)	22 (5%)	1 (0%)	56	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ILE

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	191/207 (92%)	190 (100%)	1 (0%)	94	96
1	B	172/207 (83%)	171 (99%)	1 (1%)	92	94
All	All	363/414 (88%)	361 (99%)	2 (1%)	92	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	B	274	PHE

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 ⓘ

7 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	$\# Z > 2$
2	P54	A	1	-	26,26,26	2.85	5 (19%)	36,36,36	2.29	6 (16%)
3	IPA	A	2	-	3,3,3	0.41	0	3,3,3	0.51	0
4	GOL	A	3	-	5,5,5	0.27	0	5,5,5	0.59	0
3	IPA	A	338	-	3,3,3	0.50	0	3,3,3	0.80	0
3	IPA	A	4	-	3,3,3	0.64	0	3,3,3	0.97	0
3	IPA	A	5	-	3,3,3	0.48	0	3,3,3	0.61	0
2	P54	B	1	-	26,26,26	2.50	4 (15%)	36,36,36	2.06	8 (22%)

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
2	P54	A	1	-	-	0/9/9/9	0/1/3/3
3	IPA	A	2	-	-	0/0/0/0	0/0/0/0
4	GOL	A	3	-	-	0/4/4/4	0/0/0/0
3	IPA	A	338	-	-	0/0/0/0	0/0/0/0
3	IPA	A	4	-	-	0/0/0/0	0/0/0/0
3	IPA	A	5	-	-	0/0/0/0	0/0/0/0
2	P54	B	1	-	-	0/9/9/9	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	P54	C14-C15	-9.28	1.26	1.46
2	A	1	P54	C14-C15	-8.62	1.27	1.46
2	A	1	P54	C2-N9	6.63	1.39	1.33
2	B	1	P54	C15-C16	5.55	1.30	1.17
2	A	1	P54	C15-C16	5.46	1.30	1.17
2	A	1	P54	C17-S10	-4.47	1.71	1.78
2	A	1	P54	C8-N7	4.33	1.42	1.34
2	B	1	P54	C17-S10	-4.24	1.72	1.78
2	B	1	P54	C2-N9	3.95	1.36	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	P54	C8-N9-C2	-10.06	100.50	110.31
2	B	1	P54	C8-N9-C2	-7.81	102.69	110.31
2	B	1	P54	C8-S10-C17	5.43	111.45	102.26
2	A	1	P54	C8-S10-C17	5.01	110.74	102.26
2	A	1	P54	C21-C17-S10	3.39	124.57	117.39
2	B	1	P54	C21-C17-S10	3.01	123.75	117.39
2	B	1	P54	N9-C2-N4	-2.97	126.22	128.19
2	A	1	P54	C21-C22-C20	-2.62	119.08	122.17
2	A	1	P54	C14-C13-C12	2.58	117.06	111.85
2	B	1	P54	N9-C8-N7	-2.45	115.27	118.72
2	B	1	P54	S10-C8-N9	-2.37	120.29	125.55
2	B	1	P54	C13-C14-C15	2.35	124.18	113.67
2	B	1	P54	C21-C22-C20	-2.04	119.76	122.17
2	A	1	P54	C18-C17-S10	-2.04	114.76	119.55

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	228/236 (96%)	0.66	27 (11%)	5 5	21, 43, 177, 220	0
1	B	218/236 (92%)	1.19	45 (20%)	1 2	33, 66, 169, 220	0
All	All	446/472 (94%)	0.92	72 (16%)	3 3	21, 56, 176, 220	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	MET	9.7
1	B	184	ASP	9.1
1	B	286	THR	8.4
1	B	179	THR	8.3
1	A	181	ALA	8.3
1	B	181	ALA	7.9
1	B	175	LEU	7.6
1	B	183	GLU	6.4
1	B	331	TRP	6.3
1	A	183	GLU	6.1
1	B	174	PHE	6.0
1	B	173	GLU	5.8
1	A	179	THR	5.6
1	B	185	GLY	5.5
1	B	261	LEU	5.5
1	B	274	PHE	5.4
1	B	329	THR	5.2
1	B	186	GLN	5.2
1	B	182	GLN	5.1
1	A	80	ALA	5.1
1	A	184	ASP	4.9
1	A	182	GLN	4.7
1	B	127	ALA	4.7
1	A	76	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	75	LYS	4.5
1	A	329	THR	4.4
1	B	330	VAL	4.3
1	A	286	THR	4.3
1	B	77	ALA	4.1
1	B	328	LYS	4.1
1	B	76	PHE	4.0
1	B	180	GLU	3.9
1	B	285	LYS	3.8
1	A	178	MET	3.5
1	A	180	GLU	3.5
1	A	77	ALA	3.4
1	A	169	SER	3.4
1	B	128	GLY	3.3
1	A	328	LYS	3.1
1	A	330	VAL	3.1
1	A	185	GLY	3.0
1	A	247	ILE	2.8
1	A	175	LEU	2.8
1	A	177	LYS	2.8
1	A	69	LEU	2.8
1	A	90	ILE	2.8
1	B	124	ASN	2.8
1	B	166	ILE	2.7
1	A	173	GLU	2.7
1	B	230	PHE	2.7
1	B	130	GLU	2.6
1	B	188	THR	2.6
1	A	176	ASN	2.6
1	B	126	LEU	2.5
1	B	273	GLN	2.5
1	A	187	SER	2.5
1	B	282	TRP	2.4
1	A	209	VAL	2.4
1	B	74	GLU	2.4
1	B	190	GLU	2.4
1	A	249	LEU	2.3
1	B	123	GLU	2.3
1	B	215	HIS	2.3
1	B	276	ASN	2.2
1	B	332	ASP	2.2
1	B	284	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	247	ILE	2.1
1	B	147	VAL	2.1
1	B	262	ASP	2.1
1	B	164	GLY	2.1
1	B	169	SER	2.0
1	B	168	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
4	GOL	A	3	6/6	0.39	9.99	47,48,50,52	0
3	IPA	A	338	4/4	0.13	1.65	42,43,44,50	0
2	P54	B	1	24/24	0.14	-0.15	26,33,37,39	0
2	P54	A	1	24/24	0.16	-0.16	13,20,23,24	0
3	IPA	A	4	4/4	0.15	-0.19	39,41,42,43	0
3	IPA	A	5	4/4	0.14	-0.32	42,43,45,45	0
3	IPA	A	2	4/4	0.13	-0.68	44,45,47,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.