



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:08 PM UTC

PDB ID : 1K4U / pdb_00001k4u
Title : Solution structure of the C-terminal SH3 domain of p67phox complexed with the C-terminal tail region of p47phox
Authors : Kami, K.; Takeya, R.; Sumimoto, H.; Kohda, D.
Deposited on : 2001-10-08

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

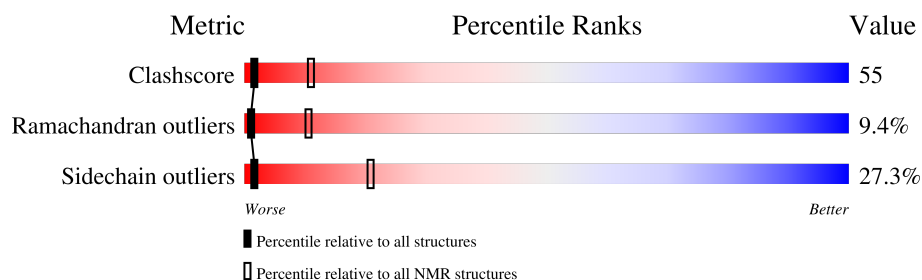
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	S	62	
2	P	32	

2 Ensemble composition and analysis

This entry contains 22 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 7 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	S:460-S:512, P:360-P:386 (80)	0.45	16

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 9 single-model clusters were found.

Cluster number	Models
1	4, 13, 14, 15, 16, 18
2	6, 9, 10, 17, 19
3	2, 11
Single-model clusters	1; 3; 5; 7; 8; 12; 20; 21; 22

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1468 atoms, of which 739 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX.

Mol	Chain	Residues	Atoms					Trace
1	S	62	Total	C	H	N	O	0
			971	314	481	74	102	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	499	SER	CYS	engineered mutation	UNP P19878
S	514	SER	CYS	engineered mutation	UNP P19878

- Molecule 2 is a protein called PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX.

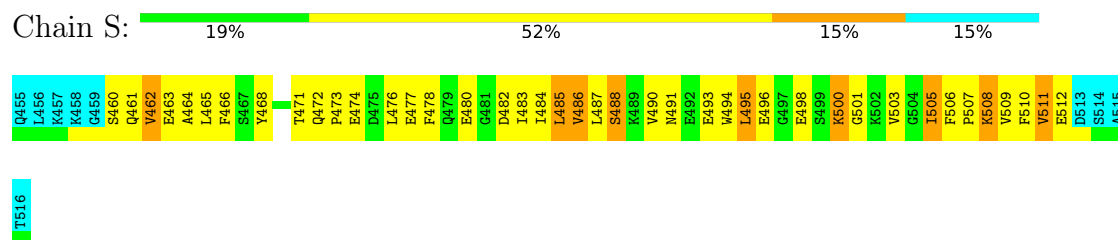
Mol	Chain	Residues	Atoms						Trace
2	P	32	Total	C	H	N	O	S	0
			497	147	258	46	45	1	

4 Residue-property plots

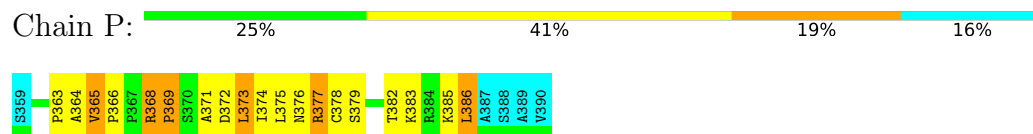
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

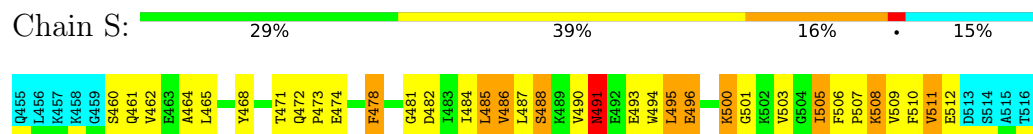


4.2 Scores per residue for each member of the ensemble

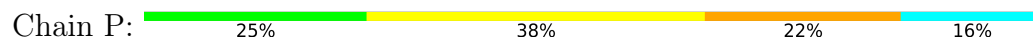
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



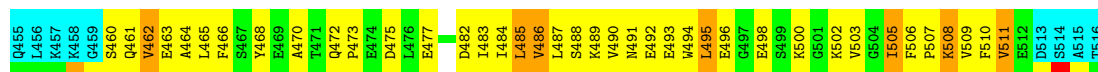
- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



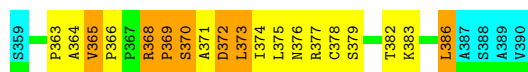
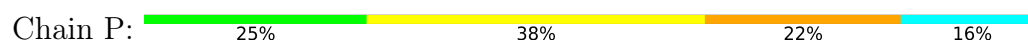


4.2.2 Score per residue for model 2

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

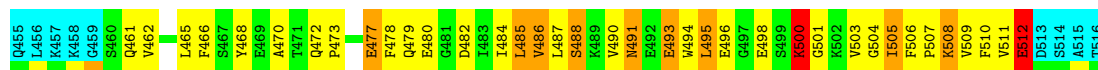


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



4.2.3 Score per residue for model 3

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



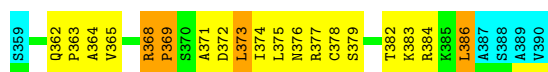
4.2.4 Score per residue for model 4

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



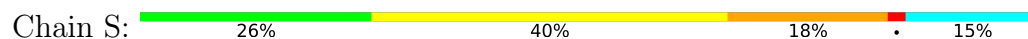
- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



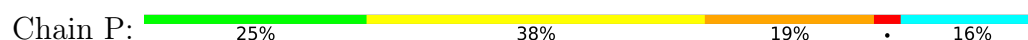


4.2.5 Score per residue for model 5

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

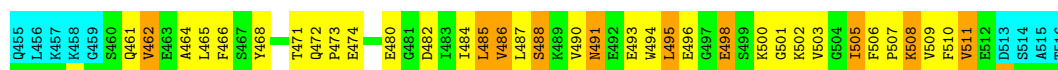


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



4.2.6 Score per residue for model 6

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

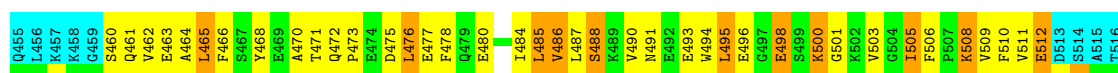
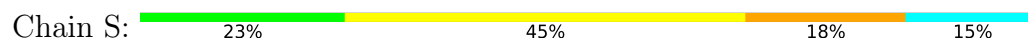


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



4.2.7 Score per residue for model 7

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



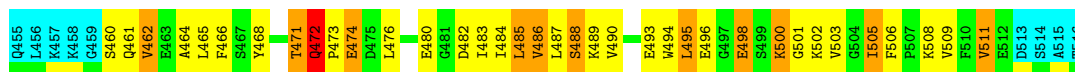
- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



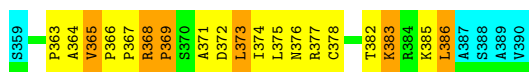
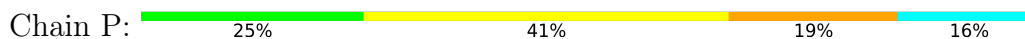


4.2.8 Score per residue for model 8

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

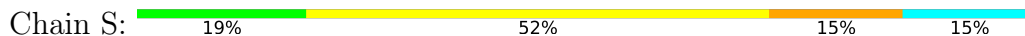


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

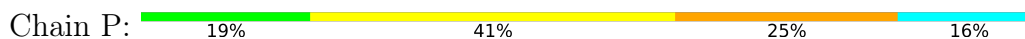


4.2.9 Score per residue for model 9

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

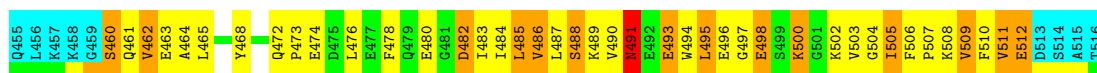
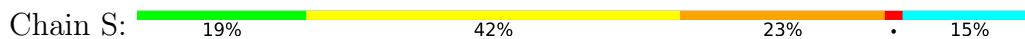


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



4.2.10 Score per residue for model 10

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



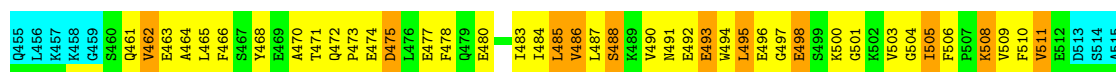
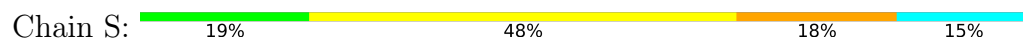
- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX





4.2.11 Score per residue for model 11

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

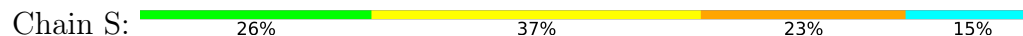


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



4.2.12 Score per residue for model 12

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX



- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

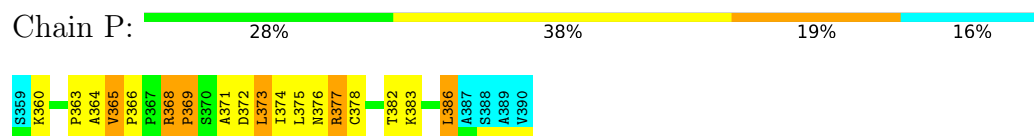


4.2.13 Score per residue for model 13

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

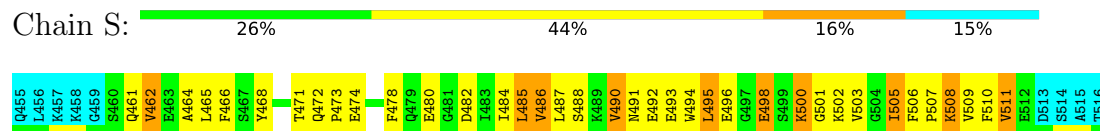


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

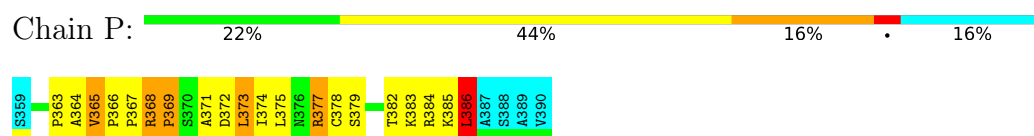


4.2.14 Score per residue for model 14

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

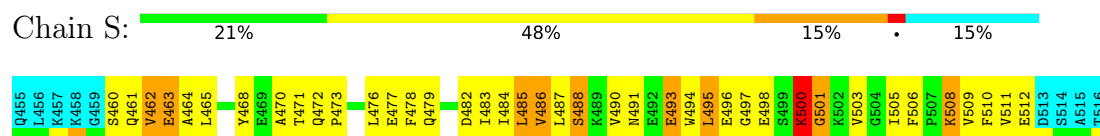


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

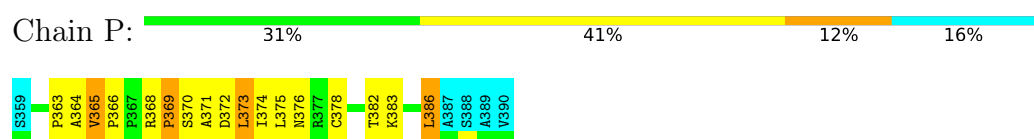


4.2.15 Score per residue for model 15

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

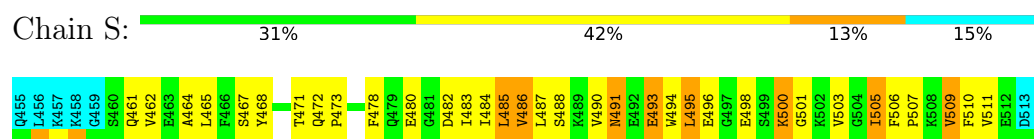


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

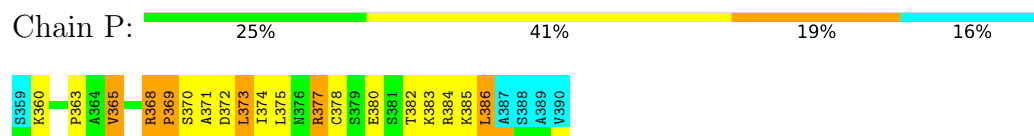


4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

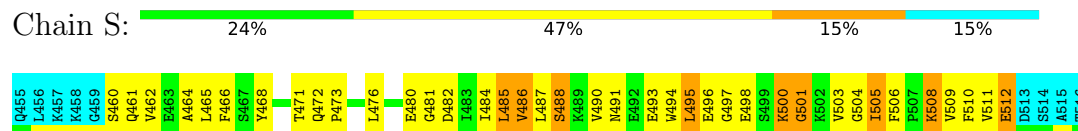


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

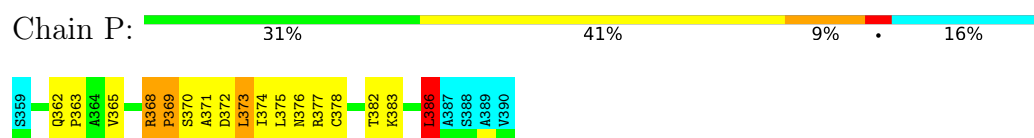


4.2.17 Score per residue for model 17

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

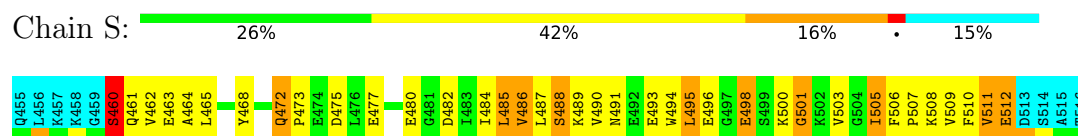


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

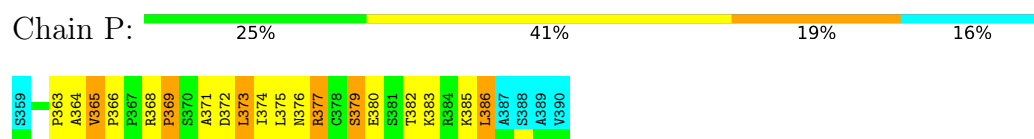


4.2.18 Score per residue for model 18

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

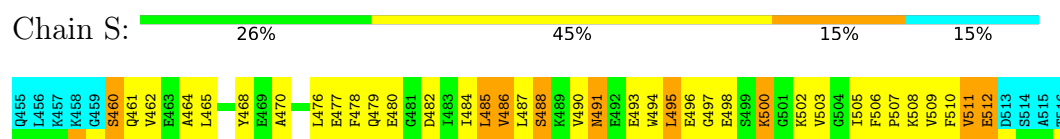


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

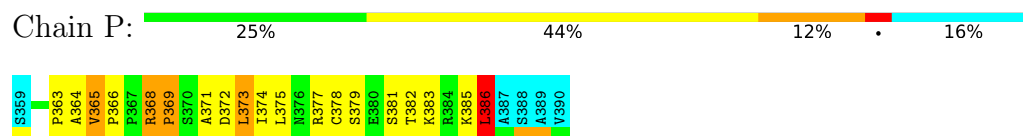


4.2.19 Score per residue for model 19

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

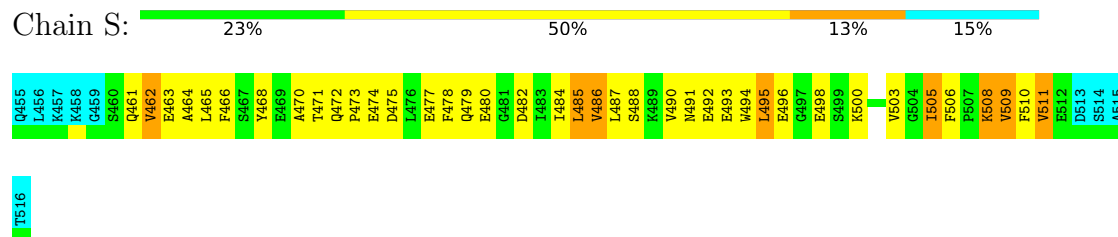


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

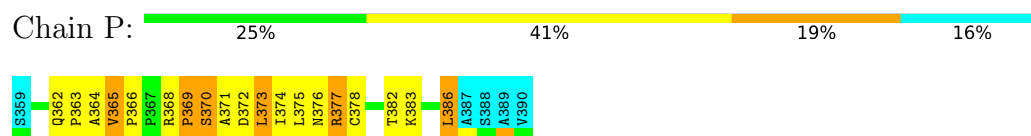


4.2.20 Score per residue for model 20

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

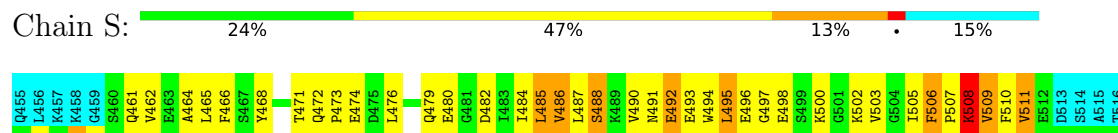


- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX

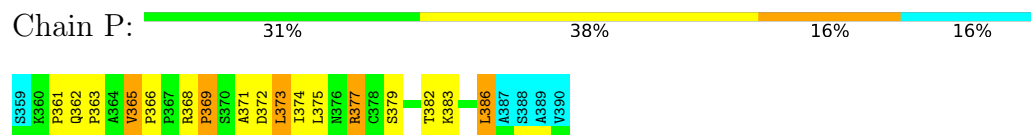


4.2.21 Score per residue for model 21

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX

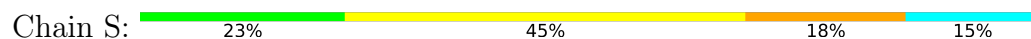


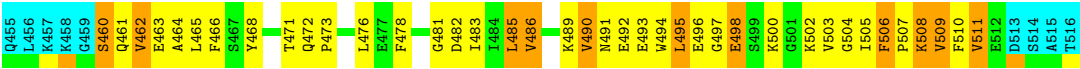
- Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



4.2.22 Score per residue for model 22

- Molecule 1: PHAGOCYTE NADPH OXIDASE SUBUNIT P67PHOX





● Molecule 2: PHAGOCYTE NADPH OXIDASE SUBUNIT P47PHOX



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 22 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	S	424	410	410	51±6
2	P	209	227	227	29±3
All	All	13926	14014	14014	1525

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 55.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:486:VAL:HG13	1:S:495:LEU:HD13	1.09	1.22	2	22
2:P:375:LEU:HD23	2:P:383:LYS:HG2	0.91	1.42	11	22
2:P:373:LEU:HD12	2:P:374:ILE:N	0.88	1.84	1	22
1:S:478:PHE:CD2	1:S:484:ILE:HD11	0.83	2.08	20	8
2:P:372:ASP:HA	2:P:375:LEU:HD12	0.83	1.50	3	22
1:S:495:LEU:HD21	1:S:508:LYS:CG	0.83	2.03	22	4
1:S:461:GLN:HA	1:S:486:VAL:HG23	0.81	1.53	11	22
2:P:369:PRO:HB3	2:P:373:LEU:HD11	0.79	1.54	15	22
1:S:503:VAL:HG12	2:P:382:THR:OG1	0.79	1.77	4	21
1:S:496:GLU:HA	1:S:505:ILE:HG22	0.78	1.52	22	22
1:S:511:VAL:O	1:S:511:VAL:HG23	0.78	1.78	1	15
1:S:462:VAL:HG21	1:S:511:VAL:HG21	0.78	1.53	17	10
1:S:509:VAL:HG13	1:S:510:PHE:CD1	0.76	2.16	22	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:486:VAL:CG1	1:S:495:LEU:HD13	0.76	2.11	16	21
1:S:485:LEU:HD13	1:S:487:LEU:CD2	0.75	2.11	12	4
1:S:485:LEU:HD13	1:S:485:LEU:O	0.75	1.82	16	21
2:P:369:PRO:CB	2:P:373:LEU:HD11	0.74	2.12	15	2
1:S:462:VAL:HG22	1:S:486:VAL:HG22	0.74	1.59	10	9
1:S:490:VAL:HG12	1:S:491:ASN:HD22	0.73	1.43	3	1
2:P:371:ALA:HB1	2:P:386:LEU:HB2	0.73	1.61	1	22
1:S:472:GLN:N	1:S:473:PRO:CD	0.72	2.52	8	1
2:P:375:LEU:HD23	2:P:383:LYS:CG	0.71	2.14	17	22
2:P:373:LEU:HD12	2:P:373:LEU:C	0.71	2.09	5	22
2:P:373:LEU:C	2:P:373:LEU:CD1	0.71	2.64	18	22
1:S:461:GLN:CA	1:S:486:VAL:HG23	0.71	2.16	12	21
1:S:485:LEU:HD13	1:S:487:LEU:HD22	0.71	1.61	12	4
1:S:464:ALA:C	1:S:465:LEU:HD12	0.70	2.11	22	18
1:S:485:LEU:C	1:S:485:LEU:HD22	0.70	2.10	14	17
1:S:487:LEU:HD12	1:S:496:GLU:OE2	0.70	1.87	1	1
1:S:484:ILE:HD12	1:S:511:VAL:CG1	0.70	2.17	21	4
1:S:495:LEU:HD21	1:S:508:LYS:HG3	0.70	1.61	22	2
1:S:507:PRO:HB2	1:S:509:VAL:HG12	0.70	1.61	22	13
1:S:468:TYR:CE1	2:P:365:VAL:HG21	0.69	2.21	1	14
1:S:490:VAL:HG11	2:P:374:ILE:HG12	0.69	1.64	21	14
1:S:462:VAL:CG2	1:S:511:VAL:HG21	0.69	2.17	17	9
1:S:484:ILE:HG21	1:S:506:PHE:CZ	0.69	2.22	13	9
1:S:505:ILE:HG23	2:P:382:THR:HG21	0.69	1.65	22	14
1:S:495:LEU:HD21	1:S:508:LYS:CD	0.69	2.17	21	2
1:S:498:GLU:HG3	1:S:503:VAL:HG22	0.68	1.65	3	5
2:P:371:ALA:O	2:P:374:ILE:HB	0.67	1.89	19	21
1:S:490:VAL:O	2:P:373:LEU:HD13	0.67	1.90	6	10
1:S:470:ALA:HB1	1:S:475:ASP:HB3	0.67	1.66	20	4
1:S:463:GLU:HG2	1:S:483:ILE:HD13	0.65	1.66	2	9
2:P:371:ALA:HA	2:P:386:LEU:HD13	0.65	1.67	13	15
1:S:462:VAL:HG22	1:S:486:VAL:CG2	0.65	2.22	1	12
1:S:476:LEU:HD22	1:S:497:GLY:HA3	0.64	1.68	21	6
1:S:498:GLU:CG	1:S:503:VAL:HG22	0.64	2.21	7	5
1:S:503:VAL:HG11	2:P:381:SER:HB2	0.63	1.68	19	1
1:S:506:PHE:CE2	1:S:511:VAL:HG11	0.63	2.29	7	4
1:S:485:LEU:HD11	1:S:487:LEU:CD2	0.63	2.23	19	11
2:P:375:LEU:HA	2:P:383:LYS:HG2	0.62	1.70	22	22
1:S:485:LEU:HD12	1:S:498:GLU:HB3	0.62	1.72	10	9
1:S:490:VAL:HG13	2:P:377:ARG:HG3	0.62	1.72	18	1
1:S:494:TRP:CD1	2:P:369:PRO:HD3	0.62	2.30	21	22

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:468:TYR:CE2	1:S:470:ALA:HB2	0.62	2.29	7	4
1:S:486:VAL:HG13	1:S:495:LEU:CD1	0.62	2.23	13	3
1:S:465:LEU:HD22	1:S:512:GLU:CG	0.61	2.25	17	1
1:S:485:LEU:HD22	1:S:486:VAL:N	0.61	2.11	5	12
1:S:463:GLU:CG	1:S:483:ILE:HD13	0.61	2.26	22	7
1:S:504:GLY:O	1:S:505:ILE:HG23	0.60	1.96	3	1
1:S:491:ASN:ND2	1:S:494:TRP:HB2	0.60	2.10	16	2
1:S:509:VAL:HG13	1:S:510:PHE:HD1	0.60	1.56	16	13
1:S:474:GLU:HG3	1:S:505:ILE:HD11	0.60	1.70	5	3
1:S:474:GLU:HB3	2:P:386:LEU:HD23	0.60	1.72	9	3
1:S:465:LEU:HD12	1:S:465:LEU:N	0.60	2.12	20	18
1:S:495:LEU:O	1:S:505:ILE:HG22	0.59	1.97	3	21
1:S:490:VAL:HG12	1:S:491:ASN:ND2	0.59	2.12	3	1
1:S:495:LEU:HD11	1:S:506:PHE:CE2	0.59	2.32	7	5
2:P:374:ILE:HG23	2:P:378:CYS:SG	0.59	2.37	9	10
1:S:465:LEU:HD22	1:S:512:GLU:HG3	0.59	1.75	17	1
1:S:494:TRP:CD1	2:P:369:PRO:CD	0.59	2.85	16	5
1:S:485:LEU:HD22	1:S:485:LEU:C	0.59	2.22	15	5
1:S:495:LEU:HD12	1:S:506:PHE:CE1	0.58	2.34	15	8
1:S:505:ILE:HD13	2:P:374:ILE:HD13	0.58	1.73	20	15
1:S:474:GLU:CG	1:S:505:ILE:HD11	0.58	2.28	8	1
1:S:464:ALA:HA	1:S:511:VAL:HG12	0.58	1.76	15	7
2:P:373:LEU:HD22	2:P:377:ARG:NH1	0.58	2.14	8	2
2:P:372:ASP:CA	2:P:375:LEU:HD12	0.57	2.27	19	22
2:P:375:LEU:HD23	2:P:383:LYS:CB	0.57	2.29	22	21
2:P:375:LEU:HG	2:P:386:LEU:HD12	0.57	1.76	10	17
1:S:487:LEU:O	1:S:488:SER:HB2	0.56	2.00	15	19
2:P:373:LEU:O	2:P:377:ARG:HG2	0.56	2.00	18	1
1:S:510:PHE:CE1	2:P:363:PRO:HG2	0.56	2.36	7	19
1:S:509:VAL:HG13	1:S:510:PHE:CE1	0.56	2.36	22	2
1:S:470:ALA:HB3	1:S:477:GLU:HB3	0.56	1.78	5	1
1:S:495:LEU:HD21	1:S:508:LYS:CB	0.56	2.31	21	10
1:S:494:TRP:CE2	2:P:368:ARG:HA	0.55	2.36	12	9
1:S:495:LEU:HD11	1:S:506:PHE:CZ	0.55	2.36	12	2
1:S:490:VAL:HG23	1:S:495:LEU:HA	0.55	1.78	4	22
1:S:490:VAL:HG11	2:P:374:ILE:CG1	0.55	2.32	21	2
1:S:511:VAL:O	1:S:511:VAL:CG2	0.54	2.53	18	6
1:S:465:LEU:HD11	1:S:511:VAL:O	0.54	2.01	9	1
1:S:485:LEU:C	1:S:485:LEU:CD2	0.54	2.80	14	5
1:S:493:GLU:O	1:S:494:TRP:CD1	0.54	2.60	22	22
1:S:511:VAL:O	1:S:512:GLU:C	0.54	2.51	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:462:VAL:HG23	1:S:462:VAL:O	0.54	2.03	5	4
1:S:471:THR:O	1:S:472:GLN:CG	0.54	2.56	8	1
1:S:484:ILE:HD12	1:S:511:VAL:HG11	0.53	1.79	21	4
2:P:368:ARG:O	2:P:369:PRO:O	0.53	2.26	10	4
1:S:505:ILE:CD1	2:P:374:ILE:HD13	0.53	2.34	2	5
1:S:511:VAL:HG23	1:S:512:GLU:N	0.53	2.19	9	1
1:S:498:GLU:HG2	1:S:503:VAL:HG22	0.53	1.79	7	1
1:S:465:LEU:HD21	1:S:512:GLU:OE2	0.53	2.03	1	1
2:P:365:VAL:HG12	2:P:366:PRO:HD2	0.53	1.80	3	16
1:S:485:LEU:HD11	1:S:487:LEU:HD23	0.53	1.81	19	8
1:S:464:ALA:HB2	1:S:484:ILE:CD1	0.52	2.34	10	2
1:S:495:LEU:CD1	1:S:506:PHE:CZ	0.52	2.92	21	15
1:S:471:THR:C	1:S:473:PRO:HD3	0.52	2.30	8	1
1:S:470:ALA:HB3	1:S:477:GLU:HB2	0.52	1.82	3	2
1:S:505:ILE:HD13	2:P:374:ILE:CD1	0.52	2.35	2	1
2:P:369:PRO:HB2	2:P:373:LEU:HD11	0.51	1.81	1	1
1:S:485:LEU:HD13	1:S:485:LEU:C	0.51	2.30	21	9
1:S:485:LEU:HD12	1:S:498:GLU:O	0.51	2.06	13	2
1:S:461:GLN:O	1:S:462:VAL:HG13	0.51	2.06	15	11
1:S:487:LEU:HD21	1:S:498:GLU:CB	0.51	2.35	14	4
1:S:465:LEU:HD13	1:S:512:GLU:HG2	0.51	1.82	17	1
1:S:462:VAL:HB	1:S:512:GLU:O	0.51	2.06	7	1
1:S:476:LEU:HD23	1:S:506:PHE:CD1	0.51	2.41	7	6
2:P:368:ARG:HG2	2:P:369:PRO:HD2	0.51	1.83	11	3
1:S:472:GLN:N	1:S:473:PRO:HD2	0.51	2.20	8	1
1:S:491:ASN:ND2	1:S:494:TRP:N	0.50	2.59	16	3
1:S:473:PRO:O	1:S:474:GLU:HB3	0.50	2.05	8	1
2:P:371:ALA:CA	2:P:386:LEU:HD13	0.50	2.36	11	7
1:S:470:ALA:CB	1:S:477:GLU:HB3	0.50	2.37	5	1
1:S:488:SER:O	1:S:495:LEU:HB2	0.50	2.06	21	2
1:S:506:PHE:CD1	1:S:506:PHE:N	0.50	2.80	22	10
1:S:494:TRP:CG	2:P:369:PRO:HD3	0.50	2.42	21	13
1:S:476:LEU:HD12	1:S:477:GLU:N	0.50	2.21	7	1
2:P:371:ALA:HA	2:P:374:ILE:HD12	0.50	1.83	21	1
2:P:370:SER:O	2:P:371:ALA:C	0.49	2.55	1	1
1:S:487:LEU:HD21	1:S:498:GLU:HB3	0.49	1.83	14	4
1:S:465:LEU:CD1	1:S:511:VAL:C	0.49	2.85	5	3
1:S:484:ILE:HG21	1:S:506:PHE:CE1	0.49	2.42	6	3
1:S:463:GLU:O	1:S:511:VAL:HB	0.49	2.08	7	1
1:S:490:VAL:O	2:P:377:ARG:HD3	0.49	2.07	21	9
1:S:474:GLU:CB	2:P:386:LEU:HD23	0.49	2.37	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:465:LEU:HD21	1:S:512:GLU:HG2	0.49	1.84	18	3
1:S:462:VAL:HG21	1:S:511:VAL:CG2	0.48	2.35	18	5
1:S:490:VAL:HG23	1:S:496:GLU:N	0.48	2.24	3	6
1:S:490:VAL:HG22	2:P:377:ARG:O	0.48	2.08	14	5
1:S:487:LEU:HB2	1:S:496:GLU:OE1	0.48	2.09	9	1
1:S:460:SER:N	1:S:486:VAL:O	0.48	2.47	19	6
1:S:465:LEU:HD13	1:S:512:GLU:CG	0.48	2.39	7	1
1:S:506:PHE:HE2	1:S:511:VAL:HG21	0.48	1.67	22	1
1:S:490:VAL:HG13	2:P:374:ILE:HA	0.48	1.85	21	4
1:S:478:PHE:N	1:S:478:PHE:CD1	0.48	2.82	1	6
2:P:375:LEU:HA	2:P:383:LYS:CG	0.48	2.39	10	11
1:S:464:ALA:HB2	1:S:484:ILE:HD12	0.48	1.85	12	1
2:P:369:PRO:HB3	2:P:373:LEU:CD1	0.47	2.39	18	2
1:S:460:SER:O	1:S:485:LEU:HD22	0.47	2.09	10	2
1:S:494:TRP:CG	2:P:369:PRO:HD2	0.47	2.44	1	1
1:S:463:GLU:HA	1:S:482:ASP:O	0.47	2.10	2	3
1:S:471:THR:O	1:S:472:GLN:CB	0.47	2.61	8	1
2:P:375:LEU:HD23	2:P:383:LYS:HB3	0.47	1.85	16	7
1:S:497:GLY:N	1:S:504:GLY:O	0.47	2.48	22	2
1:S:465:LEU:CD1	1:S:511:VAL:O	0.47	2.63	7	1
1:S:490:VAL:CG2	1:S:495:LEU:HA	0.47	2.40	21	6
1:S:464:ALA:HB3	1:S:482:ASP:H	0.47	1.69	1	14
1:S:478:PHE:CG	1:S:484:ILE:HD11	0.46	2.44	15	2
1:S:484:ILE:HG22	1:S:485:LEU:N	0.46	2.25	21	10
1:S:462:VAL:HG22	1:S:486:VAL:HG21	0.46	1.87	14	1
1:S:476:LEU:HD22	1:S:497:GLY:CA	0.46	2.40	21	1
1:S:468:TYR:C	1:S:468:TYR:CD1	0.46	2.93	3	9
1:S:462:VAL:CG2	1:S:511:VAL:CG2	0.46	2.93	15	12
1:S:495:LEU:CD1	1:S:506:PHE:CE1	0.46	2.99	3	3
1:S:507:PRO:HG2	1:S:510:PHE:CD1	0.46	2.46	1	5
2:P:385:LYS:C	2:P:386:LEU:HD23	0.46	2.36	12	4
1:S:474:GLU:CB	2:P:386:LEU:CD2	0.46	2.94	9	3
1:S:460:SER:O	1:S:486:VAL:N	0.46	2.49	13	6
1:S:506:PHE:CE2	1:S:511:VAL:CG1	0.46	2.99	7	1
2:P:373:LEU:CD1	2:P:374:ILE:N	0.46	2.72	15	1
1:S:494:TRP:CZ2	2:P:368:ARG:HD3	0.45	2.46	2	1
1:S:497:GLY:O	1:S:504:GLY:N	0.45	2.49	11	3
2:P:382:THR:O	2:P:386:LEU:HD21	0.45	2.10	19	3
1:S:478:PHE:CD2	1:S:484:ILE:CD1	0.45	2.98	9	3
1:S:508:LYS:O	1:S:511:VAL:HG22	0.45	2.11	12	1
1:S:505:ILE:CG2	2:P:378:CYS:SG	0.45	3.05	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:490:VAL:O	2:P:377:ARG:CD	0.45	2.65	3	1
1:S:493:GLU:C	1:S:494:TRP:CD1	0.45	2.95	3	2
1:S:494:TRP:CD1	2:P:369:PRO:HD2	0.45	2.46	15	4
1:S:463:GLU:O	1:S:511:VAL:CA	0.45	2.64	7	1
1:S:500:LYS:O	1:S:501:GLY:C	0.45	2.59	18	11
1:S:491:ASN:OD1	1:S:494:TRP:N	0.45	2.50	7	8
1:S:478:PHE:CE1	1:S:506:PHE:CB	0.45	3.00	1	7
1:S:496:GLU:CD	1:S:497:GLY:N	0.45	2.75	9	1
2:P:369:PRO:HB2	2:P:374:ILE:HD11	0.45	1.87	9	4
1:S:495:LEU:CD1	1:S:506:PHE:CE2	0.45	3.00	22	1
1:S:487:LEU:HD12	1:S:496:GLU:CD	0.44	2.37	1	1
2:P:371:ALA:O	2:P:386:LEU:CD1	0.44	2.65	1	1
2:P:368:ARG:CD	2:P:368:ARG:N	0.44	2.81	2	4
1:S:508:LYS:HA	1:S:511:VAL:HG22	0.44	1.88	1	4
1:S:478:PHE:CD1	1:S:478:PHE:N	0.44	2.85	11	6
1:S:487:LEU:HD13	1:S:496:GLU:OE2	0.44	2.13	7	1
1:S:506:PHE:HE2	1:S:511:VAL:HG11	0.44	1.73	15	2
2:P:385:LYS:O	2:P:386:LEU:HD23	0.44	2.11	5	2
1:S:465:LEU:CD1	1:S:511:VAL:HA	0.44	2.43	12	4
2:P:365:VAL:CG1	2:P:366:PRO:HD2	0.44	2.43	3	2
1:S:494:TRP:HA	1:S:507:PRO:HA	0.44	1.90	21	1
1:S:494:TRP:CZ2	2:P:368:ARG:CD	0.43	3.01	2	1
1:S:468:TYR:CZ	1:S:470:ALA:HB2	0.43	2.48	7	1
1:S:472:GLN:CG	1:S:475:ASP:OD2	0.43	2.66	12	2
1:S:499:SER:O	1:S:500:LYS:C	0.43	2.60	13	1
1:S:465:LEU:N	1:S:465:LEU:CD1	0.43	2.82	2	3
1:S:462:VAL:HG21	1:S:511:VAL:HG23	0.43	1.90	7	1
1:S:495:LEU:HD21	1:S:508:LYS:HB2	0.43	1.89	21	1
2:P:368:ARG:HD3	2:P:368:ARG:N	0.43	2.28	2	1
1:S:464:ALA:HB3	1:S:482:ASP:N	0.43	2.27	1	2
1:S:491:ASN:O	1:S:492:GLU:CB	0.43	2.66	21	1
1:S:494:TRP:CE3	1:S:506:PHE:C	0.43	2.96	22	1
1:S:466:PHE:N	1:S:480:GLU:HA	0.43	2.28	17	1
1:S:470:ALA:CB	1:S:477:GLU:CG	0.43	2.97	15	1
1:S:466:PHE:CE2	2:P:363:PRO:HD3	0.43	2.49	11	8
1:S:478:PHE:CE1	1:S:506:PHE:HB2	0.43	2.49	19	5
1:S:465:LEU:O	1:S:466:PHE:CD1	0.43	2.72	7	2
2:P:374:ILE:O	2:P:378:CYS:HB2	0.43	2.14	14	10
1:S:491:ASN:ND2	1:S:491:ASN:C	0.43	2.77	10	1
2:P:368:ARG:N	2:P:368:ARG:CD	0.43	2.82	6	1
1:S:493:GLU:O	1:S:507:PRO:HA	0.43	2.13	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:468:TYR:O	1:S:477:GLU:CG	0.43	2.67	2	3
2:P:370:SER:O	2:P:372:ASP:N	0.42	2.51	15	3
1:S:487:LEU:HB2	1:S:496:GLU:CG	0.42	2.43	4	2
1:S:476:LEU:O	1:S:478:PHE:CE2	0.42	2.73	5	2
1:S:490:VAL:HG23	1:S:495:LEU:C	0.42	2.39	3	2
1:S:485:LEU:CD1	1:S:487:LEU:CD2	0.42	2.94	14	3
1:S:484:ILE:HD12	1:S:484:ILE:N	0.42	2.30	17	1
1:S:476:LEU:CD2	1:S:497:GLY:HA3	0.42	2.45	10	3
1:S:468:TYR:CD1	1:S:468:TYR:C	0.42	2.97	10	3
1:S:491:ASN:O	1:S:491:ASN:CG	0.42	2.62	12	3
1:S:468:TYR:CD2	1:S:470:ALA:HB2	0.42	2.50	20	2
1:S:511:VAL:C	1:S:512:GLU:CG	0.42	2.93	12	1
1:S:473:PRO:O	2:P:385:LYS:HB3	0.41	2.15	8	1
2:P:362:GLN:HB2	2:P:363:PRO:HD2	0.41	1.92	21	1
1:S:466:PHE:CE1	2:P:363:PRO:HD3	0.41	2.51	22	1
1:S:488:SER:O	1:S:495:LEU:CB	0.41	2.69	12	3
1:S:485:LEU:HD13	1:S:487:LEU:HD21	0.41	1.88	12	1
1:S:490:VAL:O	2:P:377:ARG:NE	0.41	2.52	14	2
2:P:375:LEU:HG	2:P:386:LEU:CD1	0.41	2.46	19	1
2:P:371:ALA:HB1	2:P:386:LEU:CB	0.41	2.41	1	1
1:S:493:GLU:O	1:S:494:TRP:CG	0.41	2.74	18	2
1:S:460:SER:C	1:S:461:GLN:CG	0.41	2.94	8	2
1:S:464:ALA:C	1:S:466:PHE:H	0.41	2.22	7	1
1:S:504:GLY:CA	2:P:382:THR:OG1	0.41	2.69	9	1
1:S:490:VAL:HG12	1:S:491:ASN:N	0.41	2.30	14	1
2:P:373:LEU:O	2:P:377:ARG:CG	0.41	2.68	18	1
1:S:510:PHE:CD1	1:S:510:PHE:N	0.41	2.89	22	2
1:S:490:VAL:CG2	1:S:495:LEU:C	0.41	2.93	3	1
1:S:491:ASN:HB3	2:P:373:LEU:CD2	0.41	2.46	3	1
1:S:466:PHE:CD1	2:P:362:GLN:HA	0.41	2.51	11	4
1:S:484:ILE:CG2	1:S:485:LEU:N	0.41	2.84	11	1
2:P:373:LEU:O	2:P:377:ARG:HD2	0.41	2.16	3	1
1:S:474:GLU:HA	2:P:385:LYS:HD2	0.41	1.93	14	1
2:P:374:ILE:O	2:P:378:CYS:N	0.41	2.54	14	1
1:S:490:VAL:CG1	2:P:374:ILE:CG1	0.41	2.99	15	2
1:S:510:PHE:C	1:S:511:VAL:HG13	0.40	2.42	1	4
1:S:487:LEU:CD2	1:S:498:GLU:CB	0.40	2.99	12	1
2:P:368:ARG:CG	2:P:369:PRO:HD2	0.40	2.45	12	1
1:S:460:SER:O	1:S:486:VAL:O	0.40	2.38	13	1
1:S:494:TRP:HB2	2:P:369:PRO:HG3	0.40	1.91	1	1
2:P:369:PRO:HB2	2:P:374:ILE:CG1	0.40	2.47	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:S:507:PRO:C	1:S:509:VAL:N	0.40	2.79	21	2
1:S:494:TRP:CG	2:P:369:PRO:CD	0.40	3.04	1	1
1:S:510:PHE:CZ	2:P:363:PRO:O	0.40	2.74	19	2
1:S:461:GLN:O	1:S:462:VAL:CG1	0.40	2.70	1	1
1:S:478:PHE:CB	1:S:484:ILE:HD11	0.40	2.45	15	1
2:P:371:ALA:O	2:P:374:ILE:CB	0.40	2.66	19	1
1:S:491:ASN:CG	1:S:492:GLU:N	0.40	2.79	21	1

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	S	53/62 (85%)	39±2 (74±4%)	9±2 (17±5%)	5±2 (9±3%)	1	11
2	P	27/32 (84%)	18±1 (65±5%)	7±2 (25±6%)	3±1 (9±4%)	1	10
All	All	1760/2068 (85%)	1251 (71%)	344 (20%)	165 (9%)	1	10

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	S	473	PRO	20
2	P	369	PRO	19
1	S	511	VAL	17
1	S	488	SER	16
2	P	364	ALA	13
1	S	500	LYS	13
1	S	512	GLU	11
1	S	491	ASN	10
2	P	386	LEU	5
1	S	481	GLY	4
2	P	367	PRO	4
1	S	462	VAL	4
2	P	368	ARG	4
2	P	379	SER	3

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Mol	Chain	Res	Type	Models (Total)
2	P	380	GLU	3
1	S	490	VAL	3
1	S	501	GLY	3
2	P	361	PRO	2
1	S	463	GLU	2
2	P	360	LYS	2
2	P	371	ALA	1
1	S	465	LEU	1
1	S	472	GLN	1
1	S	474	GLU	1
1	S	460	SER	1
1	S	492	GLU	1
1	S	508	LYS	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	S	47/54 (87%)	34±2 (73±4%)	13±2 (27±4%)	2	21
2	P	25/28 (89%)	18±1 (72±6%)	7±1 (28±6%)	1	19
All	All	1584/1804 (88%)	1152 (73%)	432 (27%)	1	21

All 48 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	S	485	LEU	22
1	S	486	VAL	22
1	S	495	LEU	22
2	P	365	VAL	22
2	P	373	LEU	22
2	P	386	LEU	22
1	S	508	LYS	19
1	S	472	GLN	18
1	S	505	ILE	18
2	P	368	ARG	16
2	P	377	ARG	16

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Mol	Chain	Res	Type	Models (Total)
1	S	480	GLU	16
1	S	471	THR	15
2	P	376	ASN	15
1	S	498	GLU	14
1	S	500	LYS	12
1	S	509	VAL	12
1	S	462	VAL	11
2	P	379	SER	10
1	S	492	GLU	9
1	S	502	LYS	9
1	S	460	SER	8
2	P	385	LYS	8
1	S	489	LYS	7
1	S	493	GLU	7
1	S	474	GLU	6
1	S	479	GLN	6
2	P	384	ARG	6
2	P	370	SER	5
1	S	477	GLU	4
1	S	491	ASN	3
1	S	461	GLN	3
2	P	362	GLN	3
2	P	380	GLU	3
2	P	372	ASP	2
1	S	482	ASP	2
1	S	512	GLU	2
1	S	476	LEU	2
2	P	381	SER	2
1	S	467	SER	2
1	S	506	PHE	2
1	S	478	PHE	1
1	S	496	GLU	1
2	P	374	ILE	1
2	P	383	LYS	1
2	P	360	LYS	1
1	S	475	ASP	1
1	S	463	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided