Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 10:05 PM EST

PDB ID	:	2PQ4
Title	:	NMR solution structure of NapD in complex with NapA1-35 signal peptide
Authors	:	Minailiuc, O.M.; Ekiel, I.; Milad, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2007-05-01

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 (i) symbol.

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

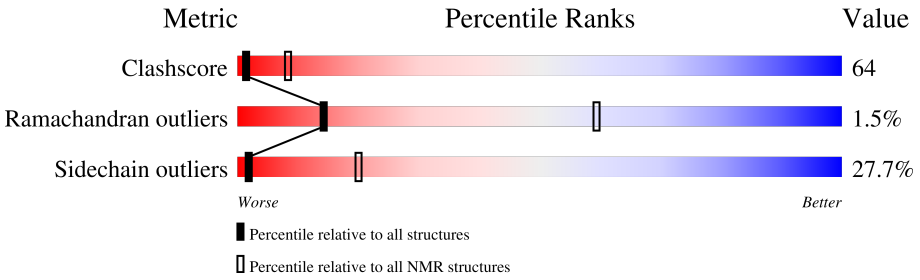
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	90	17% 56% 7% • 20%
2	B	35	26% 9% 6% 60%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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	A:9-A:80, B:10-B:23 (86)	0.17	14

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, 17, 18, 19, 20
2	1, 2, 8, 16

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1833 atoms, of which 913 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein napD.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	90	1337	419	655	115	145	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0A9I5
A	2	SER	-	expression tag	UNP P0A9I5
A	3	HIS	-	expression tag	UNP P0A9I5

- Molecule 2 is a protein called Periplasmic nitrate reductase precursor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	35	496	148	258	48	40	2	0

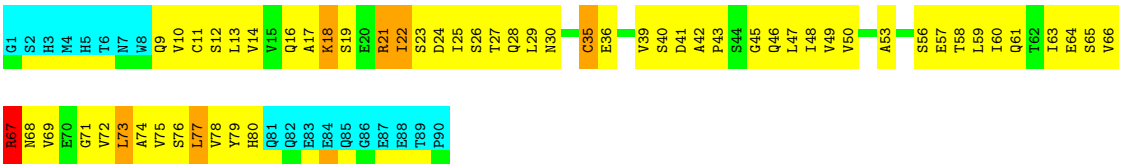
4 Residue-property plots (i)

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.

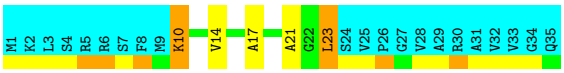
• Molecule 1: Protein napD

Chain A: 17% 56% 7% • 20%



• Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 26% 9% 6% 60%



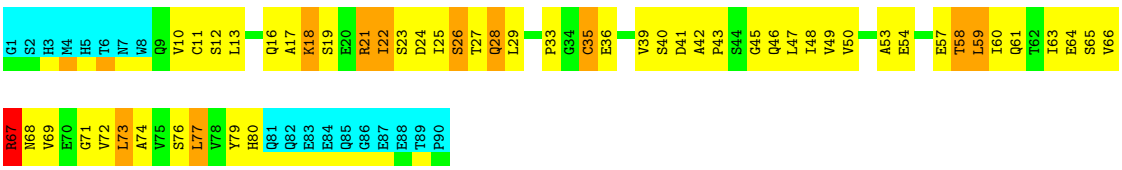
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Protein napD

Chain A: 21% 47% 11% • 20%



• Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 20% 14% • • 60%

M1 K2 L3 S4 R5 R6 S7 F8 M9 K10 A11 N12 A13 V14 A17 A21 G22 L23 S24 V25 P26 G27 V28 A29 R30 A31 V32 V33 G34 Q35

4.2.2 Score per residue for model 2

- Molecule 1: Protein napD

Chain A: 20% 43% 16% • 20%

G1 S2 H3 M4 H5 T6 N7 W8 Q9 V10 C11 S12 L13 V14 V15 Q16 A17 K18 S19 E20 R21 I22 S23 D24 I25 S26 T27 Q28 L29 N30 A31 F32 P33 G34 C35 E36 V37 A38 V39 S40 D41 A42 P43 S44 G45 Q46 L47 I48 V49 V50 V51 E52 A53 E57 T58 L59 I60 Q61 T62

I63 E64 S65 V66 R67 N68 V69 E70 G71 V72 L73 A74 V75 S76 L77 V78 Y79 H80 Q81 Q82 E83 E84 Q85 G86 E87 E88 T89 P90

- Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 20% 14% • • 60%

M1 K2 L3 S4 R5 R6 S7 F8 M9 K10 V14 A15 A16 A17 A20 A21 G22 L23 S24 V25 P26 G27 V28 A29 R30 A31 V32 V33 G34 Q35

4.2.3 Score per residue for model 3

- Molecule 1: Protein napD

Chain A: 19% 53% 7% • 20%

G1 S2 H3 M4 H5 T6 N7 W8 Q9 V10 C11 S12 L13 V14 V15 Q16 A17 K18 S19 E20 R21 I22 S23 D24 I25 S26 T27 Q28 L29 C35 S40 D41 A42 P43 S44 G45 Q46 L47 I48 V49 V50 A53 E54 D55 S56 E57 T58 L59 I60 Q61 T62 I63 E64 S65 V66 R67 N68

V69 E70 G71 V72 L73 A74 V75 S76 L77 V78 Y79 H80 Q81 Q82 E83 E84 Q85 G86 E87 E88 T89 P90

- Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 17% 17% • • 60%

M1 K2 L3 S4 R5 R6 S7 F8 M9 K10 A11 N12 A13 V14 A15 A16 A17 A20 A21 G22 L23 S24 V25 P26 G27 V28 A29 R30 A31 V32 V33 G34 Q35

4.2.4 Score per residue for model 4

- Molecule 1: Protein napD

Chain A: 21% 47% 11% • 20%

G1 S2 H3 M4 H5 T6 N7 W8 Q9 V10 C11 S12 L13 V14 V15 Q16 A17 K18 S19 E20 R21 I22 S23 D24 I25 S26 T27 Q28 L29 N30 C35 E36 V37 A38 V39 S40 D41 A42 P43 S44 G45 Q46 L47 I48 V49 V50 V51 E52 A53 E57 T58 L59 I60 Q61 T62 I63 E64 S65

V66 R67 N68 V69 E70 G71 V72 L73 A74 V75 S76 L77 V78 Y79 H80 Q81 Q82 E83 E84 Q85 G86 E87 E88 T89 P90

• Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 23% 11% • • 60%

M1 K2 L3 S4 R5 R6 S7 F8 M9 K10 A13 V14 A17 A21 G22 L23 S24 V25 P26 G27 V28 A29 R30 A31 V32 V33 G34 Q35

4.2.5 Score per residue for model 5

• Molecule 1: Protein napD

Chain A: 21% 48% 10% • 20%

G1 S2 H3 M4 H5 T6 N7 W8 C11 S12 L13 Q16 A17 K18 S19 E20 R21 I22 S23 D24 I25 S26 T27 Q28 L29 N30 C35 E36 V37 S40 D41 A42 P43 S44 G45 Q46 L47 I48 V49 V50 A53 E54 D55 S56 E57 T58 L59 I60 Q61 T62 I63 E64 S65 V66 R67

N68 V69 E70 G71 V72 L73 A74 V75 S76 L77 V78 Y79 H80 Q81 Q82 E83 E84 Q85 G86 E87 E88 T89 P90

• Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 17% 17% • • 60%

M1 K2 L3 S4 R5 R6 S7 F8 M9 K10 A11 N12 A13 V14 A15 A16 A17 A20 A21 G22 L23 S24 V25 P26 G27 V28 A29 R30 A31 V32 V33 G34 Q35

4.2.6 Score per residue for model 6

• Molecule 1: Protein napD

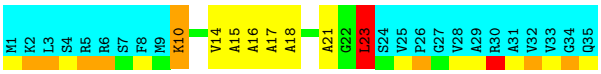
Chain A: 17% 48% 14% • 20%

G1 S2 H3 M4 H5 T6 N7 W8 Q9 V10 C11 S12 L13 V14 V15 Q16 A17 K18 S19 E20 R21 I22 S23 D24 I25 S26 T27 Q28 L29 N30 A31 F32 C35 E36 V37 S40 D41 A42 P43 S44 G45 Q46 L47 I48 V49 V50 V51 E52 A53 S56 E57 T58 L59 I60 Q61 T62 I63

E64 S65 V66 R67 N68 V69 E70 G71 V72 L73 A74 V75 S76 L77 V78 Y79 H80 Q81 Q82 E83 E84 Q85 G86 E87 E88 T89 P90

• Molecule 2: Periplasmic nitrate reductase precursor

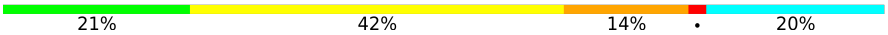
Chain B: 17% 17% • • 60%

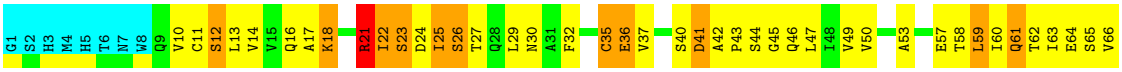


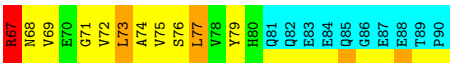
4.2.7 Score per residue for model 7

- Molecule 1: Protein napD

Chain A:

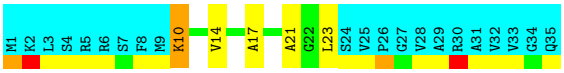






- Molecule 2: Periplasmic nitrate reductase precursor

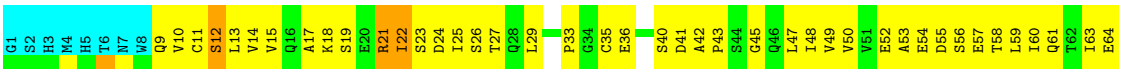
Chain B:

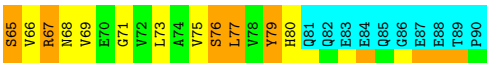


4.2.8 Score per residue for model 8

- Molecule 1: Protein napD

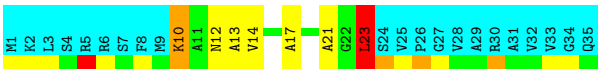
Chain A:





- Molecule 2: Periplasmic nitrate reductase precursor

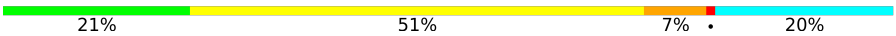
Chain B:

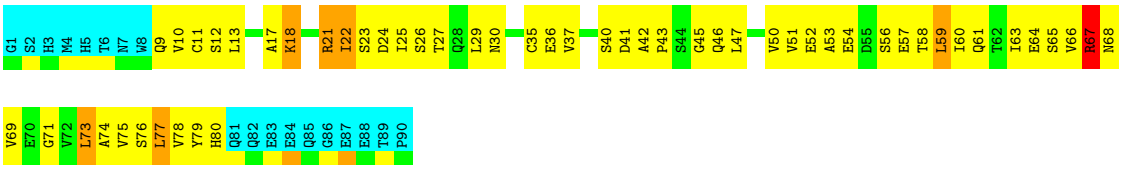


4.2.9 Score per residue for model 9

- Molecule 1: Protein napD

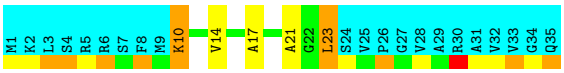
Chain A:





• Molecule 2: Periplasmic nitrate reductase precursor

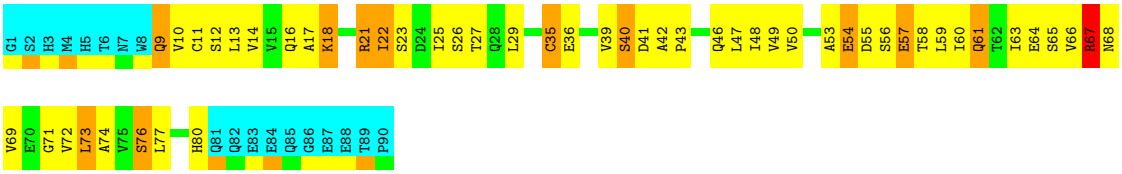
Chain B:



4.2.10 Score per residue for model 10

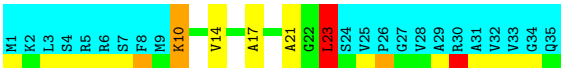
• Molecule 1: Protein napD

Chain A:



• Molecule 2: Periplasmic nitrate reductase precursor

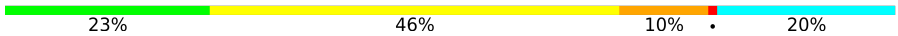
Chain B:

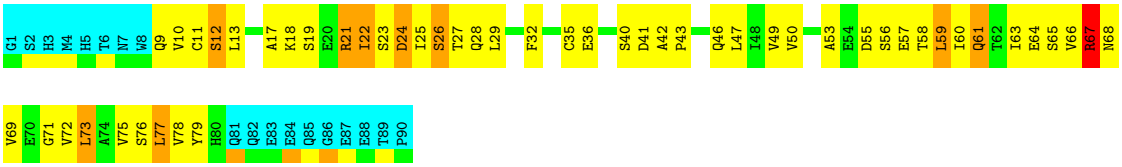


4.2.11 Score per residue for model 11

• Molecule 1: Protein napD

Chain A:



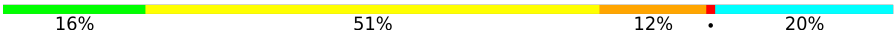


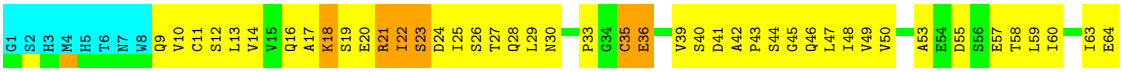
• Molecule 2: Periplasmic nitrate reductase precursor

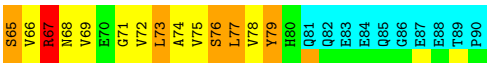
Chain B:

4.2.12 Score per residue for model 12

- Molecule 1: Protein napD

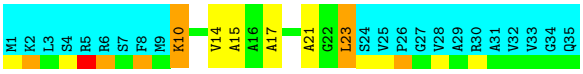
Chain A: 





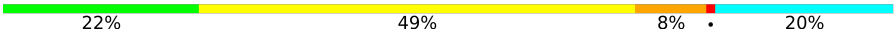
- Molecule 2: Periplasmic nitrate reductase precursor

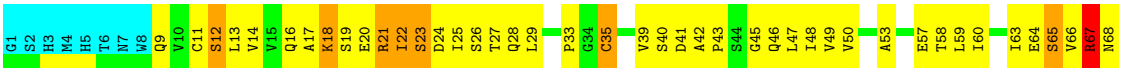
Chain B:

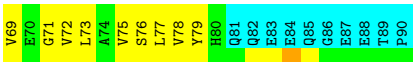


4.2.13 Score per residue for model 13

- Molecule 1: Protein napD

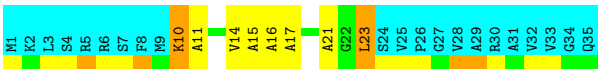
Chain A: 





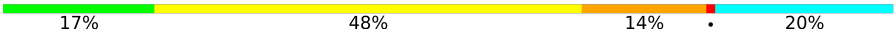
- Molecule 2: Periplasmic nitrate reductase precursor

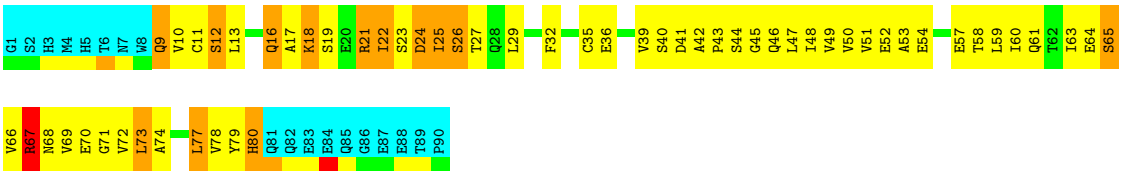
Chain B:



4.2.14 Score per residue for model 14 (medoid)

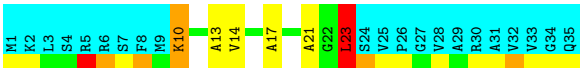
- Molecule 1: Protein napD

Chain A: 



• Molecule 2: Periplasmic nitrate reductase precursor

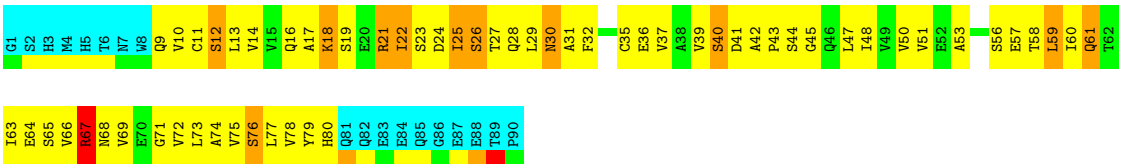
Chain B: 23% 11% • • 60%



4.2.15 Score per residue for model 15

• Molecule 1: Protein napD

Chain A: 13% 53% 12% • 20%



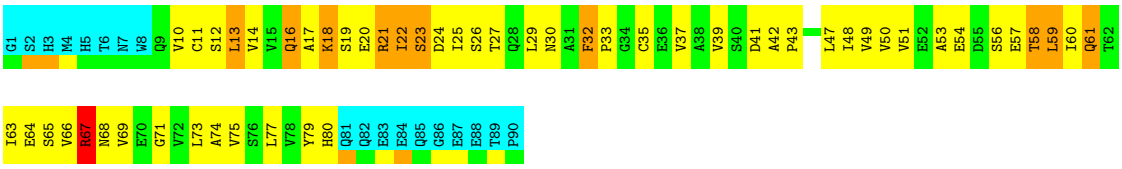
• Molecule 2: Periplasmic nitrate reductase precursor

Chain B: 20% 14% 6% 60%

4.2.16 Score per residue for model 16

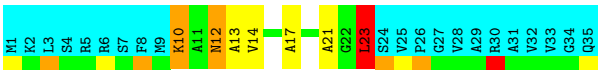
• Molecule 1: Protein napD

Chain A: 20% 48% 11% • 20%



• Molecule 2: Periplasmic nitrate reductase precursor

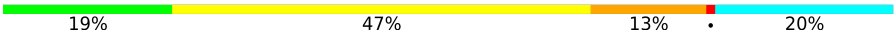
Chain B: 20% 11% 6% • 60%

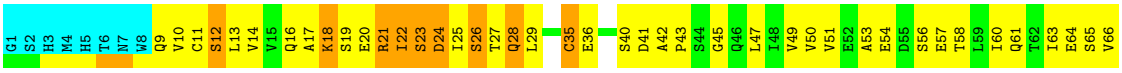


4.2.17 Score per residue for model 17

- Molecule 1: Protein napD

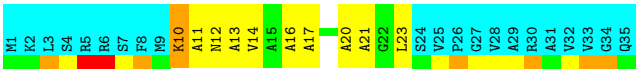
Chain A:





- Molecule 2: Periplasmic nitrate reductase precursor

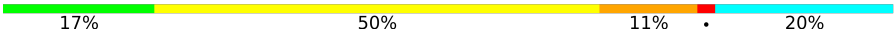
Chain B:

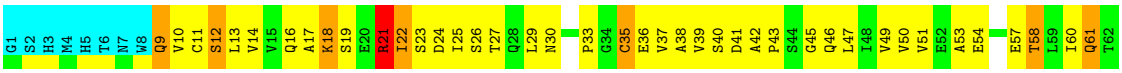


4.2.18 Score per residue for model 18

- Molecule 1: Protein napD

Chain A:





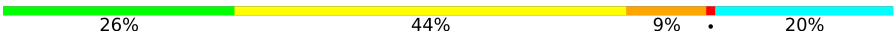
- Molecule 2: Periplasmic nitrate reductase precursor

Chain B:

4.2.19 Score per residue for model 19

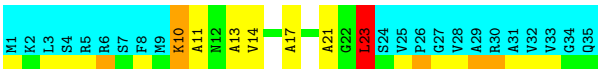
- Molecule 1: Protein napD

Chain A:



• Molecule 2: Periplasmic nitrate reductase precursor

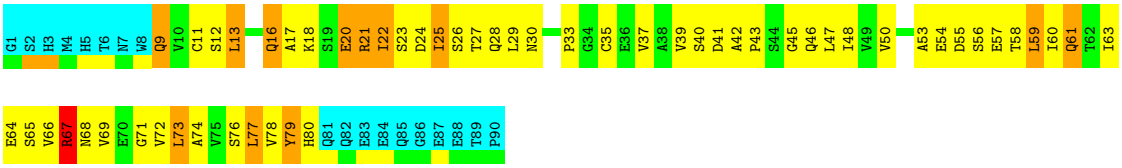
Chain B:



4.2.20 Score per residue for model 20

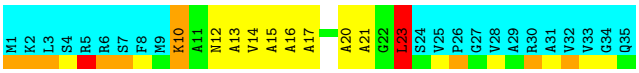
• Molecule 1: Protein napD

Chain A:



• Molecule 2: Periplasmic nitrate reductase precursor

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *CYANA2.1 TORSION ANGLE DYNAMICS*.

Of the 40 calculated structures, 20 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
CYANA	structure solution	2.1
X-PLOR-NIH NMR	refinement	2.11.2

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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	Planarity
1	A	0.0±0.0	2.0±0.0
All	All	0	40

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	21	ARG	Sidechain	20
1	A	67	ARG	Sidechain	20

6.2 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 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	A	534	537	537	75±7
2	B	81	87	87	8±3
All	All	12300	12480	12480	1593

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 64.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:HB3	1:A:22:ILE:HG23	1.05	1.24	3	20
1:A:48:ILE:HD11	2:B:23:LEU:HD22	0.95	1.36	4	12
1:A:65:SER:O	1:A:69:VAL:HG23	0.88	1.66	10	20
1:A:30:ASN:ND2	1:A:37:VAL:HG21	0.88	1.83	20	1
1:A:14:VAL:HG11	2:B:21:ALA:HB1	0.87	1.42	4	5
1:A:26:SER:OG	1:A:47:LEU:HD12	0.86	1.69	10	20
1:A:12:SER:C	1:A:13:LEU:HD13	0.83	1.93	16	1
1:A:14:VAL:HG11	2:B:21:ALA:CB	0.82	2.02	4	8
1:A:26:SER:CB	1:A:47:LEU:HD12	0.79	2.06	19	20
1:A:53:ALA:HB1	1:A:58:THR:CG2	0.79	2.07	14	9
1:A:29:LEU:HB3	1:A:49:VAL:HG21	0.78	1.55	7	12
1:A:25:ILE:HD13	1:A:69:VAL:HG11	0.77	1.54	16	18
2:B:10:LYS:O	2:B:14:VAL:HG22	0.77	1.80	18	20
1:A:11:CYS:SG	1:A:13:LEU:HD11	0.76	2.21	16	4
1:A:13:LEU:HD13	1:A:13:LEU:N	0.76	1.94	16	1
1:A:12:SER:OG	1:A:50:VAL:HG12	0.76	1.79	15	10
1:A:78:VAL:O	2:B:16:ALA:HB1	0.76	1.80	18	7
1:A:46:GLN:O	1:A:47:LEU:HD23	0.76	1.80	10	11
1:A:17:ALA:HB3	1:A:22:ILE:CG2	0.75	2.09	3	20
1:A:29:LEU:HD12	1:A:35:CYS:SG	0.75	2.21	14	17
1:A:48:ILE:HD11	2:B:23:LEU:CD2	0.75	2.12	13	7
1:A:53:ALA:HB1	1:A:58:THR:HB	0.74	1.58	6	18
1:A:13:LEU:HD23	1:A:77:LEU:CD2	0.74	2.12	14	1
1:A:13:LEU:HD23	1:A:77:LEU:CB	0.72	2.13	11	7
1:A:17:ALA:HA	1:A:73:LEU:HD23	0.72	1.61	18	12
1:A:13:LEU:HD12	1:A:13:LEU:N	0.71	2.00	3	5
1:A:60:ILE:O	1:A:63:ILE:HG22	0.70	1.87	18	20
1:A:53:ALA:HB3	1:A:59:LEU:HD12	0.70	1.62	9	9
2:B:10:LYS:O	2:B:14:VAL:HG13	0.69	1.88	2	19
1:A:13:LEU:HD12	1:A:77:LEU:HB2	0.68	1.63	16	1
1:A:13:LEU:HD23	1:A:77:LEU:HB3	0.67	1.65	20	4
2:B:17:ALA:O	2:B:21:ALA:HB3	0.66	1.89	17	20
1:A:12:SER:CB	1:A:50:VAL:HG12	0.65	2.21	11	11
1:A:12:SER:HA	1:A:50:VAL:HG12	0.65	1.67	17	14
1:A:48:ILE:HD11	2:B:23:LEU:HD23	0.65	1.68	13	1
1:A:35:CYS:SG	1:A:62:THR:HG21	0.64	2.32	7	1
1:A:48:ILE:HD13	1:A:48:ILE:N	0.64	2.08	12	1
1:A:25:ILE:HG21	1:A:69:VAL:HG11	0.63	1.69	18	10
1:A:12:SER:CA	1:A:50:VAL:HG12	0.63	2.24	17	12
1:A:16:GLN:CB	1:A:74:ALA:HB3	0.63	2.24	14	9
1:A:46:GLN:C	1:A:47:LEU:HD23	0.62	2.13	10	9
1:A:75:VAL:O	1:A:75:VAL:HG13	0.62	1.95	12	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:H	1:A:13:LEU:HD22	0.61	1.55	16	1
1:A:46:GLN:NE2	2:B:21:ALA:HB1	0.61	2.11	13	1
1:A:13:LEU:HD11	1:A:51:VAL:HG12	0.60	1.72	14	3
1:A:53:ALA:HB1	1:A:58:THR:HG21	0.60	1.71	14	2
1:A:16:GLN:HB3	1:A:74:ALA:HB3	0.60	1.73	14	10
1:A:69:VAL:CG1	1:A:72:VAL:HG23	0.60	2.27	11	15
1:A:53:ALA:CB	1:A:59:LEU:HD12	0.60	2.26	6	6
1:A:39:VAL:HG12	1:A:41:ASP:OD1	0.59	1.97	20	6
1:A:67:ARG:CD	1:A:68:ASN:N	0.59	2.66	6	16
1:A:39:VAL:HB	1:A:48:ILE:HD12	0.59	1.74	1	3
1:A:13:LEU:N	1:A:13:LEU:CD1	0.59	2.64	16	5
1:A:42:ALA:N	1:A:43:PRO:CD	0.58	2.65	7	20
1:A:30:ASN:OD1	1:A:37:VAL:HG11	0.58	1.99	20	1
1:A:53:ALA:CB	1:A:58:THR:CG2	0.58	2.81	14	2
1:A:11:CYS:SG	1:A:59:LEU:HD23	0.58	2.39	9	4
1:A:77:LEU:HD12	1:A:77:LEU:O	0.57	1.98	16	1
1:A:16:GLN:CG	1:A:74:ALA:HB3	0.57	2.30	14	6
1:A:36:GLU:C	1:A:49:VAL:HG23	0.56	2.19	7	1
1:A:13:LEU:HD23	1:A:77:LEU:HD13	0.56	1.77	9	2
1:A:22:ILE:O	1:A:26:SER:CB	0.56	2.54	17	20
1:A:16:GLN:CD	1:A:74:ALA:HB3	0.56	2.21	1	2
1:A:37:VAL:HG23	1:A:37:VAL:O	0.56	1.99	9	6
1:A:14:VAL:HG22	1:A:48:ILE:HD12	0.56	1.77	12	1
1:A:46:GLN:CG	2:B:23:LEU:CD1	0.56	2.84	13	1
1:A:13:LEU:N	1:A:13:LEU:HD22	0.56	2.16	16	1
1:A:13:LEU:CD1	1:A:51:VAL:HG12	0.55	2.31	17	4
1:A:12:SER:OG	1:A:79:TYR:CD2	0.55	2.57	12	4
1:A:17:ALA:CA	1:A:73:LEU:HD23	0.55	2.31	18	1
1:A:77:LEU:CD1	1:A:77:LEU:O	0.55	2.55	14	1
1:A:13:LEU:HD23	1:A:77:LEU:HD22	0.55	1.76	14	5
1:A:16:GLN:HG2	1:A:74:ALA:HB3	0.55	1.79	3	5
1:A:26:SER:HB3	1:A:47:LEU:HD12	0.55	1.79	15	15
1:A:26:SER:HB2	1:A:47:LEU:HD12	0.55	1.78	19	2
1:A:12:SER:OG	1:A:79:TYR:CD1	0.55	2.58	14	1
1:A:30:ASN:OD1	1:A:37:VAL:CG1	0.55	2.55	20	1
1:A:23:SER:O	1:A:27:THR:CG2	0.54	2.56	1	20
1:A:49:VAL:HG13	1:A:49:VAL:O	0.54	2.03	17	10
2:B:16:ALA:O	2:B:20:ALA:HB3	0.54	2.02	3	5
1:A:30:ASN:OD1	1:A:30:ASN:N	0.54	2.40	20	1
1:A:77:LEU:O	1:A:77:LEU:HD12	0.54	2.03	14	1
1:A:22:ILE:O	1:A:26:SER:N	0.54	2.41	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ASP:O	1:A:47:LEU:CD2	0.53	2.57	7	20
1:A:77:LEU:O	1:A:77:LEU:CG	0.53	2.56	16	4
1:A:13:LEU:CD2	1:A:77:LEU:HD13	0.53	2.33	9	1
1:A:18:LYS:CB	1:A:21:ARG:CG	0.53	2.87	1	20
1:A:63:ILE:O	1:A:67:ARG:CG	0.53	2.57	19	13
1:A:11:CYS:CB	1:A:79:TYR:O	0.52	2.57	16	4
1:A:53:ALA:CB	1:A:58:THR:HG22	0.52	2.33	14	1
1:A:30:ASN:OD1	1:A:31:ALA:N	0.52	2.43	15	1
1:A:56:SER:O	1:A:60:ILE:HG23	0.52	2.04	9	4
1:A:68:ASN:OD1	1:A:69:VAL:N	0.52	2.42	17	1
1:A:30:ASN:ND2	1:A:37:VAL:CG2	0.52	2.67	20	2
1:A:57:GLU:O	1:A:60:ILE:CG1	0.52	2.57	8	13
1:A:64:GLU:HA	1:A:67:ARG:CG	0.52	2.35	18	20
1:A:39:VAL:HG12	1:A:41:ASP:OD2	0.52	2.03	15	3
1:A:14:VAL:HG23	1:A:76:SER:O	0.52	2.04	13	5
1:A:14:VAL:CG2	1:A:76:SER:O	0.52	2.58	13	5
2:B:10:LYS:O	2:B:14:VAL:CG2	0.52	2.58	2	12
1:A:61:GLN:O	1:A:64:GLU:CG	0.52	2.58	7	11
1:A:18:LYS:HB2	1:A:21:ARG:CG	0.52	2.35	17	20
1:A:30:ASN:CG	1:A:37:VAL:HG22	0.52	2.25	7	2
1:A:11:CYS:SG	1:A:59:LEU:HD21	0.52	2.45	20	1
1:A:48:ILE:CD1	2:B:23:LEU:HD22	0.52	2.24	4	4
1:A:66:VAL:HG23	1:A:67:ARG:N	0.51	2.20	12	20
1:A:9:GLN:NE2	1:A:54:GLU:O	0.51	2.43	20	3
1:A:47:LEU:C	1:A:48:ILE:HD13	0.51	2.26	12	1
1:A:78:VAL:O	2:B:16:ALA:CB	0.51	2.57	18	2
1:A:25:ILE:O	1:A:29:LEU:CD2	0.51	2.59	10	19
2:B:10:LYS:O	2:B:14:VAL:CG1	0.51	2.58	2	3
1:A:9:GLN:OE1	1:A:56:SER:N	0.51	2.43	15	1
1:A:15:VAL:HG23	1:A:49:VAL:CG1	0.51	2.35	8	1
1:A:11:CYS:SG	1:A:59:LEU:CD2	0.51	2.99	9	4
1:A:29:LEU:H	1:A:29:LEU:HD22	0.51	1.66	20	1
1:A:42:ALA:N	1:A:43:PRO:HD3	0.50	2.22	7	1
2:B:10:LYS:HG2	2:B:14:VAL:HG13	0.50	1.83	18	1
1:A:65:SER:O	1:A:69:VAL:CG2	0.50	2.57	19	13
1:A:25:ILE:CG1	1:A:26:SER:N	0.50	2.74	5	2
1:A:55:ASP:N	1:A:55:ASP:OD1	0.50	2.44	5	4
1:A:46:GLN:HG3	2:B:23:LEU:CD1	0.50	2.36	13	1
1:A:77:LEU:O	1:A:77:LEU:CD1	0.50	2.59	16	1
1:A:29:LEU:HD22	1:A:29:LEU:N	0.50	2.22	20	20
1:A:35:CYS:SG	1:A:49:VAL:CG2	0.50	2.99	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:CB	1:A:22:ILE:HG23	0.50	2.17	15	17
1:A:41:ASP:C	1:A:43:PRO:CD	0.50	2.80	12	19
1:A:26:SER:O	1:A:30:ASN:OD1	0.50	2.30	20	1
1:A:30:ASN:ND2	1:A:37:VAL:HG11	0.49	2.21	20	1
1:A:67:ARG:HD2	1:A:68:ASN:N	0.49	2.22	6	6
1:A:75:VAL:O	1:A:75:VAL:CG1	0.49	2.60	12	4
1:A:12:SER:OG	1:A:79:TYR:CG	0.49	2.66	16	1
1:A:30:ASN:CG	1:A:37:VAL:HG11	0.49	2.27	20	1
1:A:48:ILE:N	1:A:48:ILE:CD1	0.49	2.71	12	1
1:A:26:SER:OG	1:A:47:LEU:CD1	0.49	2.58	8	4
1:A:12:SER:HB3	1:A:50:VAL:HG12	0.49	1.82	12	3
1:A:32:PHE:CG	1:A:33:PRO:HD2	0.49	2.43	16	2
1:A:25:ILE:HD13	1:A:69:VAL:CG1	0.48	2.37	20	1
1:A:12:SER:OG	1:A:50:VAL:CG1	0.48	2.61	8	5
1:A:79:TYR:CE1	2:B:13:ALA:HA	0.48	2.44	20	8
2:B:14:VAL:O	2:B:18:ALA:CB	0.48	2.62	6	2
1:A:39:VAL:HG21	1:A:48:ILE:HD12	0.48	1.86	10	1
1:A:53:ALA:HB3	1:A:59:LEU:CD1	0.47	2.39	10	2
1:A:63:ILE:O	1:A:67:ARG:HG2	0.47	2.09	19	2
1:A:13:LEU:CD2	1:A:77:LEU:CB	0.47	2.90	11	3
1:A:21:ARG:NH2	1:A:24:ASP:HB2	0.47	2.24	16	1
1:A:21:ARG:CZ	1:A:71:GLY:HA3	0.47	2.39	8	15
1:A:25:ILE:HG13	1:A:26:SER:N	0.47	2.24	5	2
1:A:18:LYS:CB	1:A:21:ARG:HB2	0.47	2.39	16	20
1:A:63:ILE:HD11	1:A:75:VAL:HG21	0.47	1.85	12	1
1:A:27:THR:O	1:A:30:ASN:OD1	0.47	2.33	15	1
1:A:49:VAL:O	1:A:49:VAL:CG1	0.47	2.62	4	5
1:A:48:ILE:CD1	2:B:23:LEU:CD2	0.47	2.90	13	1
1:A:65:SER:O	1:A:68:ASN:OD1	0.47	2.32	17	1
1:A:9:GLN:HG3	1:A:53:ALA:O	0.47	2.10	20	1
1:A:41:ASP:C	1:A:43:PRO:HD3	0.47	2.31	1	19
1:A:17:ALA:O	1:A:45:GLY:O	0.47	2.33	1	15
1:A:67:ARG:HD3	1:A:68:ASN:N	0.47	2.25	11	4
1:A:63:ILE:HD12	1:A:66:VAL:HG21	0.47	1.87	12	1
1:A:40:SER:OG	1:A:40:SER:O	0.46	2.33	7	1
1:A:13:LEU:O	1:A:49:VAL:HG12	0.46	2.10	18	1
1:A:66:VAL:O	1:A:72:VAL:CB	0.46	2.63	1	4
1:A:48:ILE:HD11	2:B:23:LEU:CD1	0.46	2.39	12	1
1:A:67:ARG:CD	1:A:67:ARG:C	0.46	2.84	20	6
1:A:25:ILE:HG21	1:A:69:VAL:CG1	0.46	2.41	7	2
1:A:39:VAL:HG22	2:B:10:LYS:CG	0.46	2.40	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:O	1:A:23:SER:OG	0.46	2.34	3	1
1:A:79:TYR:CD1	2:B:13:ALA:HA	0.46	2.46	18	2
1:A:12:SER:OG	1:A:79:TYR:CB	0.46	2.64	16	2
1:A:40:SER:O	1:A:41:ASP:OD1	0.46	2.34	17	1
1:A:46:GLN:OE1	2:B:21:ALA:O	0.46	2.34	4	1
1:A:9:GLN:CG	1:A:53:ALA:O	0.46	2.64	20	1
1:A:40:SER:O	1:A:40:SER:OG	0.46	2.33	13	5
1:A:61:GLN:O	1:A:64:GLU:HG3	0.46	2.11	7	4
1:A:79:TYR:CE2	2:B:13:ALA:HA	0.46	2.46	14	1
1:A:27:THR:HA	1:A:30:ASN:OD1	0.46	2.10	20	1
1:A:17:ALA:HA	1:A:71:GLY:O	0.45	2.11	13	20
1:A:57:GLU:O	1:A:60:ILE:HG12	0.45	2.11	3	19
1:A:60:ILE:HG13	1:A:61:GLN:N	0.45	2.26	4	16
1:A:53:ALA:N	1:A:59:LEU:CD1	0.45	2.79	6	1
1:A:11:CYS:HB2	1:A:79:TYR:O	0.45	2.11	16	7
1:A:22:ILE:O	1:A:26:SER:HB2	0.45	2.10	7	4
1:A:63:ILE:O	1:A:67:ARG:HG3	0.45	2.11	18	13
1:A:20:GLU:O	1:A:20:GLU:OE1	0.45	2.34	20	1
1:A:61:GLN:O	1:A:64:GLU:OE2	0.45	2.34	6	1
1:A:17:ALA:O	1:A:18:LYS:C	0.45	2.55	11	20
1:A:21:ARG:NE	1:A:71:GLY:HA3	0.45	2.27	3	15
1:A:39:VAL:CB	1:A:48:ILE:HD12	0.45	2.41	13	2
1:A:41:ASP:O	1:A:47:LEU:HD23	0.45	2.12	2	7
1:A:53:ALA:CB	1:A:58:THR:HB	0.45	2.42	3	13
1:A:30:ASN:CG	1:A:37:VAL:CG1	0.45	2.85	20	1
1:A:33:PRO:O	1:A:36:GLU:OE2	0.45	2.34	18	2
1:A:22:ILE:HG21	1:A:45:GLY:O	0.45	2.10	18	2
1:A:29:LEU:CB	1:A:49:VAL:HG21	0.45	2.37	17	1
1:A:64:GLU:OE1	1:A:67:ARG:NH1	0.45	2.49	20	1
1:A:44:SER:CB	1:A:46:GLN:OE1	0.45	2.65	5	1
1:A:29:LEU:HB3	1:A:49:VAL:CG2	0.45	2.42	12	1
1:A:79:TYR:CD2	2:B:13:ALA:HA	0.45	2.46	14	1
1:A:63:ILE:O	1:A:66:VAL:HG22	0.45	2.12	17	13
1:A:30:ASN:O	1:A:30:ASN:OD1	0.45	2.35	19	2
1:A:39:VAL:CG2	1:A:48:ILE:HD12	0.45	2.42	10	1
1:A:24:ASP:O	1:A:27:THR:HG22	0.44	2.12	5	15
1:A:18:LYS:CB	1:A:21:ARG:HG2	0.44	2.42	9	10
1:A:26:SER:OG	1:A:27:THR:N	0.44	2.50	20	3
1:A:53:ALA:HB1	1:A:58:THR:CB	0.44	2.39	18	4
1:A:11:CYS:O	1:A:50:VAL:HA	0.44	2.12	10	8
1:A:13:LEU:HD23	1:A:77:LEU:HD23	0.44	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:SER:OG	1:A:48:ILE:CG2	0.44	2.65	19	1
1:A:51:VAL:HG13	1:A:59:LEU:HG	0.44	1.90	9	2
1:A:13:LEU:HD12	1:A:13:LEU:H	0.44	1.71	15	2
1:A:12:SER:HB2	1:A:79:TYR:CD2	0.44	2.47	8	3
1:A:77:LEU:O	1:A:77:LEU:HG	0.44	2.13	16	3
1:A:30:ASN:HB2	1:A:37:VAL:CG2	0.44	2.43	5	6
1:A:16:GLN:O	1:A:73:LEU:N	0.44	2.49	10	3
1:A:16:GLN:HG2	1:A:73:LEU:HD11	0.44	1.89	18	1
1:A:22:ILE:O	1:A:26:SER:HB3	0.44	2.12	8	3
1:A:18:LYS:O	1:A:22:ILE:HG12	0.43	2.13	9	20
1:A:41:ASP:O	1:A:43:PRO:HD2	0.43	2.13	9	17
1:A:64:GLU:O	1:A:68:ASN:CB	0.43	2.66	5	1
1:A:12:SER:OG	1:A:79:TYR:HB3	0.43	2.13	5	3
1:A:69:VAL:HG12	1:A:72:VAL:HG23	0.43	1.90	11	1
1:A:60:ILE:O	1:A:63:ILE:CG2	0.43	2.64	6	5
1:A:25:ILE:O	1:A:28:GLN:HB2	0.43	2.14	20	2
1:A:37:VAL:O	1:A:37:VAL:CG2	0.43	2.66	9	3
1:A:67:ARG:NE	1:A:68:ASN:HB2	0.43	2.28	8	1
1:A:67:ARG:CZ	1:A:67:ARG:HB2	0.43	2.42	19	1
1:A:18:LYS:HB3	1:A:21:ARG:HG2	0.43	1.91	19	20
2:B:10:LYS:HG2	2:B:14:VAL:CG1	0.43	2.43	18	2
1:A:9:GLN:NE2	1:A:80:HIS:NE2	0.43	2.67	14	1
1:A:73:LEU:HG	1:A:74:ALA:N	0.43	2.29	17	4
1:A:61:GLN:O	1:A:64:GLU:CD	0.43	2.57	5	7
1:A:23:SER:O	1:A:27:THR:HB	0.43	2.14	5	20
1:A:10:VAL:HB	1:A:52:GLU:CB	0.43	2.43	2	2
1:A:22:ILE:O	1:A:26:SER:OG	0.43	2.33	18	1
2:B:10:LYS:CD	2:B:10:LYS:C	0.42	2.87	5	1
1:A:65:SER:OG	1:A:66:VAL:N	0.42	2.52	9	2
1:A:61:GLN:O	1:A:64:GLU:HG2	0.42	2.14	6	7
1:A:24:ASP:OD1	1:A:24:ASP:N	0.42	2.52	20	1
1:A:36:GLU:N	1:A:50:VAL:O	0.42	2.53	12	1
1:A:16:GLN:HG2	1:A:73:LEU:CD1	0.42	2.44	18	2
1:A:30:ASN:HB2	1:A:37:VAL:CG1	0.42	2.45	6	1
1:A:76:SER:HB3	2:B:21:ALA:HB2	0.42	1.91	12	1
1:A:13:LEU:N	1:A:13:LEU:CD2	0.42	2.80	16	1
1:A:9:GLN:OE1	1:A:55:ASP:HA	0.42	2.15	12	1
1:A:79:TYR:OH	2:B:12:ASN:HB3	0.42	2.15	1	2
1:A:55:ASP:OD1	1:A:55:ASP:C	0.42	2.58	3	1
2:B:14:VAL:O	2:B:18:ALA:HB3	0.42	2.15	6	2
1:A:76:SER:O	1:A:76:SER:OG	0.41	2.38	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:N	1:A:49:VAL:O	0.41	2.41	10	1
1:A:66:VAL:O	1:A:72:VAL:HG21	0.41	2.15	1	1
1:A:11:CYS:SG	1:A:13:LEU:CD1	0.41	3.04	13	1
1:A:44:SER:OG	1:A:46:GLN:OE1	0.41	2.34	14	1
1:A:48:ILE:HD11	2:B:23:LEU:HD13	0.41	1.92	14	1
1:A:14:VAL:HB	1:A:76:SER:O	0.41	2.15	15	7
1:A:78:VAL:O	1:A:79:TYR:HB2	0.41	2.15	12	6
1:A:13:LEU:HA	1:A:77:LEU:CB	0.41	2.46	7	2
1:A:15:VAL:CG2	1:A:49:VAL:HG11	0.41	2.45	8	1
2:B:11:ALA:O	2:B:14:VAL:CG2	0.41	2.68	15	4
1:A:77:LEU:C	1:A:78:VAL:HG23	0.41	2.34	20	2
1:A:21:ARG:NH1	1:A:71:GLY:N	0.41	2.68	2	2
2:B:16:ALA:O	2:B:20:ALA:CB	0.41	2.68	3	1
1:A:66:VAL:CG2	1:A:67:ARG:N	0.41	2.83	12	2
1:A:21:ARG:NH2	1:A:69:VAL:CG1	0.41	2.83	7	1
1:A:30:ASN:HB2	1:A:37:VAL:HG22	0.41	1.92	9	2
1:A:77:LEU:HG	1:A:77:LEU:O	0.41	2.16	12	3
1:A:11:CYS:HA	1:A:79:TYR:O	0.41	2.16	19	1
1:A:44:SER:O	1:A:44:SER:OG	0.41	2.39	2	1
1:A:63:ILE:HA	1:A:66:VAL:HG22	0.41	1.92	13	12
1:A:57:GLU:O	1:A:61:GLN:OE1	0.41	2.39	18	2
1:A:64:GLU:HA	1:A:67:ARG:HG2	0.41	1.93	2	8
1:A:26:SER:OG	1:A:47:LEU:HB2	0.41	2.16	6	2
1:A:29:LEU:HD22	1:A:29:LEU:H	0.41	1.76	10	5
1:A:14:VAL:CB	1:A:76:SER:O	0.41	2.69	13	1
1:A:14:VAL:HG22	1:A:48:ILE:HG12	0.40	1.91	16	1
1:A:64:GLU:O	1:A:68:ASN:HB3	0.40	2.16	16	1
1:A:66:VAL:O	1:A:72:VAL:HG11	0.40	2.16	18	1
1:A:39:VAL:HB	1:A:48:ILE:CG1	0.40	2.46	12	1
1:A:16:GLN:HA	1:A:46:GLN:CB	0.40	2.47	13	1
1:A:10:VAL:HG23	1:A:51:VAL:O	0.40	2.16	16	1
1:A:67:ARG:O	1:A:67:ARG:NH2	0.40	2.49	19	1
1:A:21:ARG:NH1	1:A:24:ASP:HB3	0.40	2.31	11	1
1:A:35:CYS:SG	1:A:49:VAL:HG21	0.40	2.56	14	1
1:A:27:THR:CG2	1:A:28:GLN:N	0.40	2.84	1	1
1:A:41:ASP:HB3	1:A:43:PRO:HD3	0.40	1.93	7	1
1:A:54:GLU:O	1:A:55:ASP:CG	0.40	2.60	10	1

6.3 Torsion angles (i)

6.3.1 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 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	A	72/90 (80%)	65±1 (90±1%)	7±1 (10±1%)	0±1 (1±1%)	26 73
2	B	14/35 (40%)	13±0 (93±0%)	0±0 (2±3%)	1±0 (5±3%)	3 23
All	All	1720/2500 (69%)	1552 (90%)	143 (8%)	25 (1%)	14 59

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	23	LEU	15
1	A	79	TYR	5
1	A	33	PRO	4
1	A	75	VAL	1

6.3.2 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 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	A	63/79 (80%)	47±2 (74±4%)	16±2 (26±4%)	2 23
2	B	4/21 (19%)	2±1 (41±14%)	2±1 (59±14%)	0 0
All	All	1340/2000 (67%)	969 (72%)	371 (28%)	2 20

All 39 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	A	22	ILE	20
1	A	73	LEU	20
2	B	10	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	67	ARG	19
1	A	77	LEU	19
2	B	23	LEU	19
1	A	59	LEU	17
1	A	19	SER	16
1	A	18	LYS	15
1	A	76	SER	15
1	A	80	HIS	14
1	A	35	CYS	13
1	A	40	SER	12
1	A	9	GLN	11
1	A	28	GLN	10
1	A	36	GLU	10
1	A	26	SER	9
1	A	61	GLN	9
1	A	12	SER	9
1	A	23	SER	8
1	A	32	PHE	8
2	B	12	ASN	8
1	A	54	GLU	7
1	A	25	ILE	7
1	A	58	THR	6
1	A	16	GLN	6
1	A	56	SER	6
1	A	20	GLU	6
1	A	65	SER	6
1	A	24	ASP	6
1	A	44	SER	5
1	A	41	ASP	2
1	A	57	GLU	2
1	A	21	ARG	2
1	A	52	GLU	2
1	A	30	ASN	2
1	A	13	LEU	2
1	A	55	ASP	2
1	A	70	GLU	1

6.3.3 RNA (i)

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 monosaccharides 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 (i)

No chemical shift data were provided