Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 07:35 AM EDT

PDB ID	:	1GHK
Title	:	SOLUTION STRUCTURE OF THE LIPOYL DOMAIN OF THE 2-OXOGLUTARATE DEHYDROGENASE COMPLEX FROM AZOTOBACTER VINELAND II, NMR, 25 STRUCTURES
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Deposited on	:	1996-01-16

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

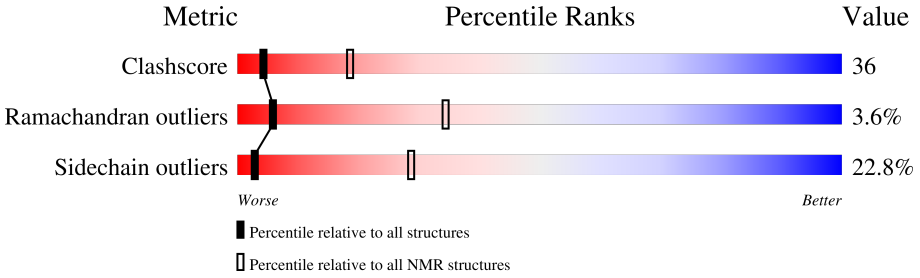
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	79	38% 48% 9% 5%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:2-A:76 (75)	0.73	4

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 7, 8, 9, 10, 14, 15, 16, 17, 19, 22, 23
2	11, 21, 24
3	1, 12, 25
4	5, 18, 20
Single-model clusters	2; 13

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1181 atoms, of which 596 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	79	1181	369	596	93	122	1	0

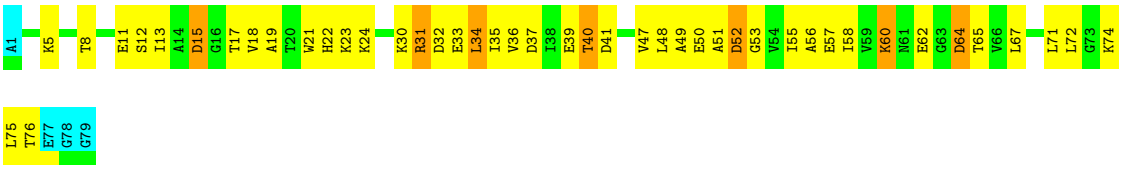
4 Residue-property plots (i)

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: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 38% 48% 9% 5%



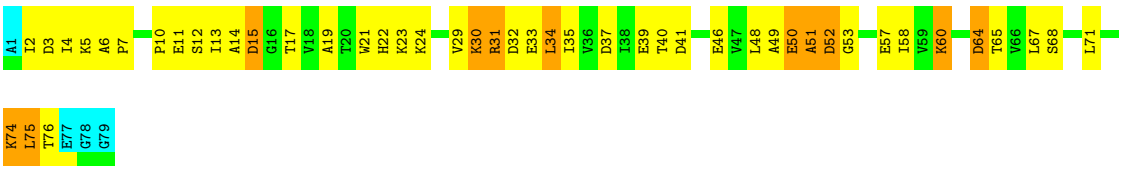
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 35% 46% 14% 5%



4.2.2 Score per residue for model 2

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 33% 49% 13% 5%

A1 I2 D3 I4 K5 A6 P7 T8 F9 P10 E11 S12 I13 A14 D15 V18 A19 T20 W21 H22 K23 K24 P25 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 M45 E46 V47 L48 A49 E50 A51 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66

L67 L71 T76 E77 G78 G79

4.2.3 Score per residue for model 3

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 29% 47% 18% • 5%

A1 I4 K5 A6 P7 P10 E11 S12 I13 A14 D15 G16 T17 V18 A19 T20 W21 H22 K23 K24 P25 G26 E27 A28 V29 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 V47 L48 A49 E50 A51 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66

L67 E70 L71 K74 L75 T76 E77 G78 G79

4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 37% 46% 9% • 5%

A1 K5 A6 P7 T8 E11 S12 I13 A14 D15 V18 A19 T20 W21 H22 K23 K24 E27 A28 V29 K30 R31 D32 E33 L34 D37 T40 D41 M45 L48 A49 E50 A51 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66 L67 S68 L71

L72 G73 K74 L75 T76 E77 G78 G79

4.2.5 Score per residue for model 5

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 46% 35% 14% 5%

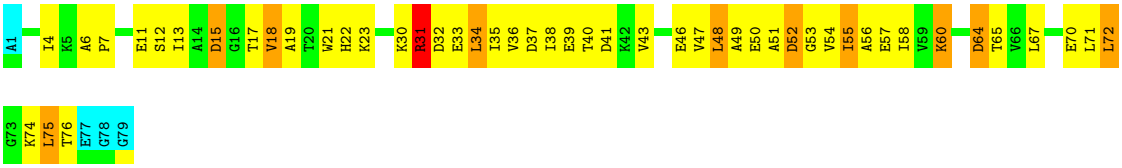
A1 I4 K5 T8 F9 P10 E11 S12 D15 G16 T17 V18 A19 T20 W21 H22 K23 K24 V29 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 K42 V43 V44 L48 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66 L67 K74

E77 G78 G79

4.2.6 Score per residue for model 6

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

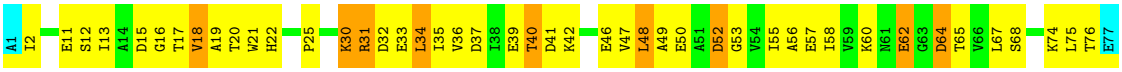
Chain A: 33% 48% 13% • 5%



4.2.7 Score per residue for model 7

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

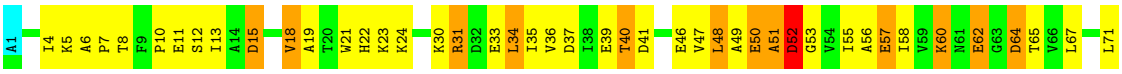
Chain A: 38% 46% 11% 5%



4.2.8 Score per residue for model 8

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

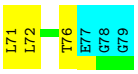
Chain A: 34% 44% 15% • 5%



4.2.9 Score per residue for model 9

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 35% 47% 10% • 5%



4.2.10 Score per residue for model 10

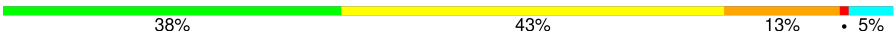
• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

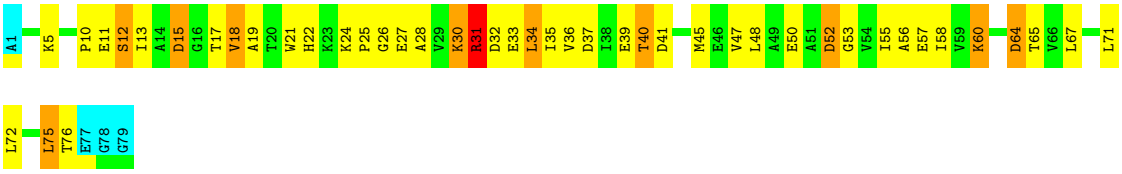
Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A:

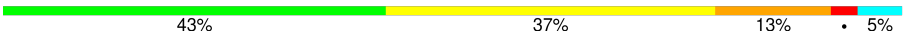


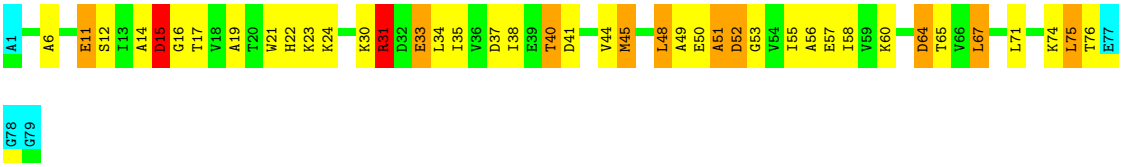


4.2.12 Score per residue for model 12

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A:





4.2.13 Score per residue for model 13

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 27% 54% 13% • 5%

A1 I2 D3 I4 K5 T8 F9 P10 E11 S12 I13 A14 D15 G16 T17 V18 A19 T20 W21 H22 K23 K24 P25 G26 E27 A28 V29 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 V44 M45 E46 V47 L48 A49 E50 A51 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66 L67 L71 L72 G73 K74 L75 T76 E77 G78 G79

4.2.14 Score per residue for model 14

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 34% 46% 15% 5%

A1 I2 D3 I4 K5 T8 E11 S12 I13 A14 D15 G16 T17 V18 A19 T20 W21 H22 K23 E27 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 K42 V43 V44 M45 E46 V47 L48 A49 E50 A51 D52 G53 V54 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66 L67 E70 L71 L75 T76 E77 G78 G79

4.2.15 Score per residue for model 15

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 37% 46% 11% • 5%

A1 I2 D3 I4 K5 A6 P7 T8 F9 P10 E11 S12 D15 G16 T17 V18 A19 T20 W21 H22 K23 K24 P25 V29 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 K42 V43 V47 L48 A49 E50 A51 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 V66 L67 L72 L75 T76 E77 G78 G79

4.2.16 Score per residue for model 16

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

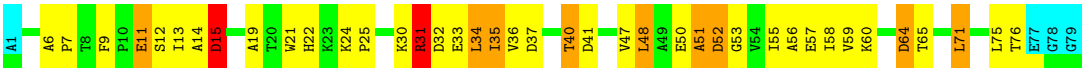
Chain A: 33% 52% 10% 5%

A1 T8 F9 P10 E11 S12 I13 A14 D15 G16 T17 V18 A19 T20 W21 H22 K23 K24 E27 A28 V29 K30 R31 D32 E33 L34 I35 V36 D37 I38 E39 T40 D41 K42 V47 L48 A49 E50 A51 D52 G53 V54 I55 A56 E57 I58 V59 K60 N61 E62 G63 D64 T65 S68 L72 G73 K74 L75 T76 E77 G78 G79

4.2.17 Score per residue for model 17

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

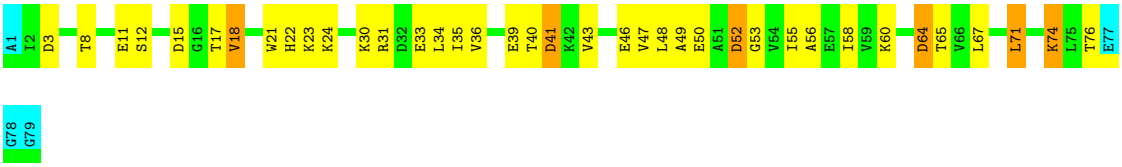
Chain A: 44% 37% 11% • 5%



4.2.18 Score per residue for model 18

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 47% 41% 8% 5%



4.2.19 Score per residue for model 19

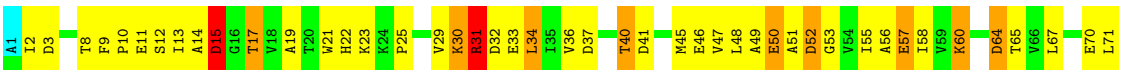
• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

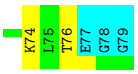
Chain A: 38% 43% 14% 5%

4.2.20 Score per residue for model 20

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A: 35% 46% 11% • 5%

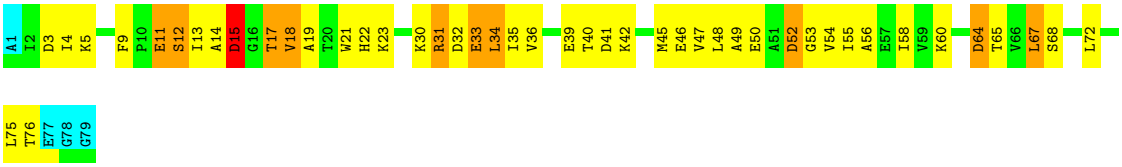




4.2.21 Score per residue for model 21

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

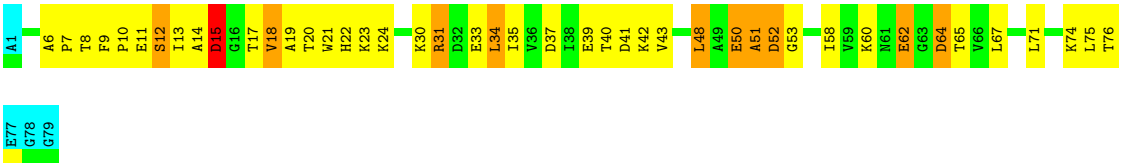
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

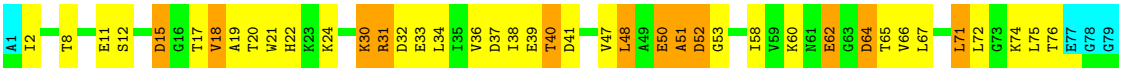
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

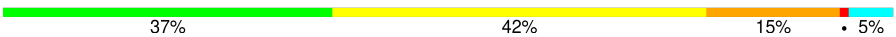
Chain A:

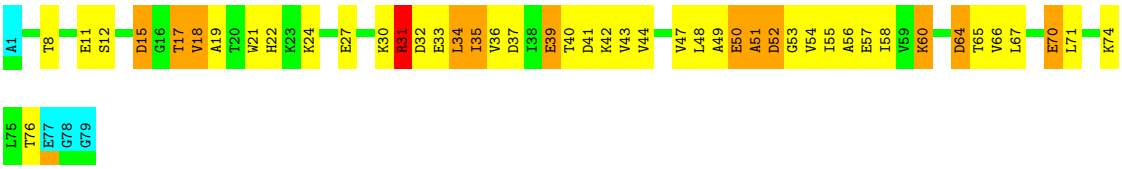


4.2.24 Score per residue for model 24

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A:





4.2.25 Score per residue for model 25

• Molecule 1: E2, THE DIHYDROLIPOAMIDE SUCCINYLTRANSFERASE COMPONENT OF 2-OXOGLUTARATE DEHYDROGENASE COMPLEX

Chain A:

5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 25 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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	1.0±0.2
All	All	0	24

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	31	ARG	Sidechain	24

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	563	577	577	41±7
All	All	14075	14425	14425	1017

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HD11	1:A:49:ALA:HB2	1.05	1.22	3	11
1:A:3:ASP:OD1	1:A:71:LEU:HD11	0.88	1.68	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG21	1:A:55:ILE:HD11	0.84	1.47	10	1
1:A:48:LEU:HD23	1:A:49:ALA:O	0.81	1.75	21	1
1:A:25:PRO:HD3	1:A:58:ILE:HD11	0.81	1.50	10	5
1:A:59:VAL:HG21	1:A:71:LEU:HD23	0.81	1.51	17	1
1:A:22:HIS:NE2	1:A:34:LEU:HD21	0.79	1.93	4	23
1:A:55:ILE:HD13	1:A:75:LEU:HD12	0.79	1.53	16	3
1:A:59:VAL:HG23	1:A:72:LEU:O	0.78	1.77	10	2
1:A:16:GLY:O	1:A:65:THR:HG23	0.78	1.77	10	3
1:A:55:ILE:HD13	1:A:75:LEU:CD1	0.77	2.09	13	2
1:A:22:HIS:CE1	1:A:34:LEU:HD21	0.77	2.15	10	21
1:A:17:THR:HG23	1:A:64:ASP:O	0.77	1.80	11	13
1:A:34:LEU:O	1:A:35:ILE:HD13	0.76	1.81	11	5
1:A:60:LYS:HG2	1:A:66:VAL:HG12	0.75	1.59	25	2
1:A:21:TRP:CZ2	1:A:58:ILE:HG23	0.74	2.17	15	6
1:A:55:ILE:HD13	1:A:55:ILE:N	0.73	1.99	10	3
1:A:38:ILE:O	1:A:44:VAL:HG23	0.72	1.84	10	1
1:A:48:LEU:HD23	1:A:48:LEU:N	0.72	2.00	9	5
1:A:75:LEU:HD23	1:A:76:THR:O	0.71	1.85	3	6
1:A:54:VAL:O	1:A:76:THR:HG22	0.71	1.85	13	3
1:A:35:ILE:HD11	1:A:49:ALA:CB	0.71	2.16	21	5
1:A:13:ILE:HG21	1:A:40:THR:CG2	0.70	2.16	16	1
1:A:25:PRO:CD	1:A:58:ILE:HD11	0.69	2.17	17	3
1:A:35:ILE:HD11	1:A:49:ALA:CA	0.69	2.17	8	1
1:A:27:GLU:O	1:A:54:VAL:HG13	0.69	1.88	4	2
1:A:21:TRP:CH2	1:A:58:ILE:HD12	0.68	2.24	8	19
1:A:32:ASP:HA	1:A:48:LEU:HD21	0.68	1.66	21	2
1:A:2:ILE:HD13	1:A:75:LEU:CD2	0.67	2.19	13	1
1:A:13:ILE:HG21	1:A:40:THR:HG22	0.67	1.65	16	2
1:A:3:ASP:OD1	1:A:71:LEU:HD12	0.67	1.89	25	1
1:A:29:VAL:HG21	1:A:35:ILE:HD11	0.67	1.66	5	1
1:A:34:LEU:HD13	1:A:46:GLU:HB3	0.67	1.67	18	1
1:A:71:LEU:C	1:A:71:LEU:HD23	0.66	2.11	10	6
1:A:35:ILE:CD1	1:A:49:ALA:HB2	0.66	2.21	18	3
1:A:32:ASP:C	1:A:48:LEU:HD21	0.65	2.11	3	1
1:A:50:GLU:O	1:A:51:ALA:HB2	0.64	1.92	14	17
1:A:21:TRP:CH2	1:A:58:ILE:CD1	0.64	2.81	9	19
1:A:22:HIS:CE1	1:A:34:LEU:CD2	0.64	2.81	10	21
1:A:71:LEU:HD11	1:A:74:LYS:HD2	0.62	1.69	8	1
1:A:17:THR:HG22	1:A:64:ASP:O	0.62	1.93	20	3
1:A:40:THR:HG23	1:A:41:ASP:N	0.62	2.10	18	4
1:A:75:LEU:HD23	1:A:76:THR:N	0.61	2.10	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:N	1:A:48:LEU:HD11	0.61	2.09	20	1
1:A:40:THR:HG22	1:A:43:VAL:O	0.61	1.96	14	4
1:A:56:ALA:HB3	1:A:74:LYS:HG2	0.60	1.72	3	1
1:A:71:LEU:HD11	1:A:74:LYS:HG3	0.59	1.73	23	1
1:A:13:ILE:HG22	1:A:15:ASP:O	0.59	1.98	21	5
1:A:59:VAL:CG2	1:A:71:LEU:HD23	0.58	2.28	17	1
1:A:34:LEU:N	1:A:48:LEU:HD12	0.58	2.13	21	1
1:A:22:HIS:NE2	1:A:34:LEU:CD2	0.58	2.67	13	24
1:A:2:ILE:HD13	1:A:75:LEU:HD23	0.57	1.76	13	1
1:A:29:VAL:HG12	1:A:30:LYS:N	0.56	2.16	15	2
1:A:8:THR:HG23	1:A:8:THR:O	0.56	2.01	23	3
1:A:19:ALA:HB3	1:A:37:ASP:CB	0.56	2.30	17	17
1:A:59:VAL:HG21	1:A:71:LEU:CD2	0.56	2.28	17	1
1:A:6:ALA:HB1	1:A:7:PRO:HD2	0.55	1.79	10	10
1:A:66:VAL:O	1:A:67:LEU:HD23	0.55	2.01	13	1
1:A:32:ASP:CA	1:A:48:LEU:HD21	0.55	2.31	21	1
1:A:55:ILE:HG22	1:A:56:ALA:N	0.55	2.17	11	15
1:A:48:LEU:N	1:A:48:LEU:CD2	0.55	2.68	7	5
1:A:34:LEU:HA	1:A:48:LEU:HD12	0.55	1.79	4	3
1:A:13:ILE:HG22	1:A:15:ASP:H	0.54	1.61	17	5
1:A:71:LEU:HD11	1:A:74:LYS:CD	0.54	2.33	8	1
1:A:9:PHE:CE2	1:A:15:ASP:C	0.53	2.81	13	2
1:A:60:LYS:HE2	1:A:66:VAL:HG12	0.53	1.78	14	1
1:A:18:VAL:HG12	1:A:19:ALA:N	0.53	2.19	7	18
1:A:55:ILE:CG2	1:A:56:ALA:N	0.53	2.72	11	7
1:A:71:LEU:HD23	1:A:72:LEU:N	0.53	2.18	10	1
1:A:50:GLU:O	1:A:51:ALA:CB	0.53	2.57	4	10
1:A:36:VAL:HG12	1:A:47:VAL:HB	0.53	1.81	21	5
1:A:66:VAL:HG11	1:A:72:LEU:HD21	0.53	1.80	4	2
1:A:13:ILE:CG2	1:A:15:ASP:O	0.53	2.57	21	7
1:A:56:ALA:CB	1:A:74:LYS:O	0.52	2.57	6	5
1:A:17:THR:CG2	1:A:64:ASP:O	0.52	2.57	21	6
1:A:19:ALA:HB3	1:A:37:ASP:O	0.52	2.04	5	6
1:A:60:LYS:CD	1:A:64:ASP:OD2	0.52	2.57	14	2
1:A:33:GLU:N	1:A:48:LEU:CD2	0.52	2.73	2	1
1:A:66:VAL:C	1:A:67:LEU:HD12	0.52	2.24	2	1
1:A:60:LYS:CG	1:A:64:ASP:OD2	0.52	2.57	5	2
1:A:16:GLY:HA2	1:A:40:THR:HG23	0.52	1.79	7	1
1:A:70:GLU:OE2	1:A:72:LEU:HD23	0.52	2.03	9	1
1:A:3:ASP:OD2	1:A:71:LEU:CD1	0.52	2.57	14	3
1:A:3:ASP:OD1	1:A:71:LEU:CD1	0.52	2.58	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ASP:C	1:A:38:ILE:HD13	0.52	2.25	3	1
1:A:17:THR:O	1:A:39:GLU:CG	0.52	2.57	7	2
1:A:14:ALA:O	1:A:15:ASP:CB	0.52	2.57	12	9
1:A:31:ARG:O	1:A:32:ASP:CB	0.52	2.58	3	18
1:A:64:ASP:OD1	1:A:65:THR:N	0.52	2.43	3	4
1:A:4:ILE:O	1:A:4:ILE:HG22	0.52	2.04	8	2
1:A:17:THR:O	1:A:39:GLU:CB	0.52	2.58	11	3
1:A:64:ASP:CG	1:A:65:THR:N	0.52	2.64	9	25
1:A:11:GLU:O	1:A:13:ILE:CD1	0.52	2.57	2	1
1:A:55:ILE:N	1:A:55:ILE:CD1	0.52	2.68	10	2
1:A:52:ASP:CG	1:A:53:GLY:N	0.51	2.64	6	25
1:A:60:LYS:HB2	1:A:72:LEU:HD23	0.51	1.82	21	1
1:A:42:LYS:O	1:A:43:VAL:CG2	0.51	2.57	14	4
1:A:56:ALA:CB	1:A:74:LYS:CG	0.51	2.88	18	1
1:A:34:LEU:N	1:A:48:LEU:CD1	0.51	2.74	21	1
1:A:60:LYS:CG	1:A:64:ASP:OD1	0.51	2.59	21	4
1:A:29:VAL:CG1	1:A:30:LYS:N	0.51	2.74	15	1
1:A:21:TRP:CZ2	1:A:58:ILE:HD12	0.51	2.41	9	18
1:A:3:ASP:OD2	1:A:5:LYS:CG	0.51	2.59	15	1
1:A:9:PHE:CE2	1:A:15:ASP:HA	0.51	2.41	22	3
1:A:43:VAL:HG12	1:A:44:VAL:N	0.51	2.20	5	1
1:A:34:LEU:O	1:A:35:ILE:CD1	0.50	2.57	11	1
1:A:38:ILE:HG22	1:A:39:GLU:N	0.50	2.21	23	1
1:A:3:ASP:OD1	1:A:4:ILE:N	0.50	2.44	21	2
1:A:58:ILE:HG23	1:A:72:LEU:O	0.50	2.07	8	3
1:A:9:PHE:CD2	1:A:15:ASP:HA	0.50	2.41	15	3
1:A:4:ILE:HD12	1:A:74:LYS:CA	0.50	2.37	6	1
1:A:11:GLU:CG	1:A:12:SER:N	0.50	2.74	6	4
1:A:56:ALA:CB	1:A:74:LYS:HG3	0.50	2.36	18	3
1:A:22:HIS:NE2	1:A:34:LEU:HD23	0.50	2.21	6	3
1:A:33:GLU:N	1:A:48:LEU:HD23	0.49	2.22	2	1
1:A:35:ILE:HD11	1:A:49:ALA:N	0.49	2.22	8	1
1:A:4:ILE:HD12	1:A:74:LYS:HA	0.49	1.83	6	1
1:A:3:ASP:OD2	1:A:71:LEU:HD12	0.49	2.07	10	1
1:A:38:ILE:HD11	1:A:47:VAL:HG22	0.49	1.85	16	1
1:A:33:GLU:C	1:A:48:LEU:CD1	0.49	2.81	23	2
1:A:29:VAL:HG22	1:A:30:LYS:N	0.49	2.21	1	1
1:A:29:VAL:HG22	1:A:53:GLY:O	0.49	2.08	9	2
1:A:11:GLU:HG3	1:A:12:SER:N	0.48	2.23	6	2
1:A:15:ASP:N	1:A:15:ASP:OD1	0.48	2.46	1	1
1:A:56:ALA:HB3	1:A:74:LYS:O	0.48	2.07	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LYS:HZ2	1:A:72:LEU:HD23	0.48	1.67	6	1
1:A:60:LYS:CD	1:A:64:ASP:OD1	0.48	2.62	6	1
1:A:59:VAL:CG2	1:A:72:LEU:O	0.48	2.57	10	1
1:A:7:PRO:O	1:A:9:PHE:CE1	0.48	2.67	17	1
1:A:44:VAL:HG13	1:A:44:VAL:O	0.48	2.08	13	2
1:A:6:ALA:HB3	1:A:67:LEU:O	0.48	2.08	12	1
1:A:27:GLU:CD	1:A:27:GLU:N	0.48	2.67	14	1
1:A:60:LYS:HD2	1:A:66:VAL:HG12	0.48	1.84	19	1
1:A:42:LYS:O	1:A:43:VAL:HG23	0.47	2.08	14	2
1:A:19:ALA:HB3	1:A:37:ASP:C	0.47	2.29	5	7
1:A:38:ILE:CG2	1:A:39:GLU:N	0.47	2.76	23	1
1:A:42:LYS:C	1:A:43:VAL:CG2	0.47	2.82	24	1
1:A:9:PHE:CZ	1:A:16:GLY:HA3	0.47	2.44	13	1
1:A:34:LEU:HD12	1:A:48:LEU:HD22	0.47	1.84	23	1
1:A:54:VAL:O	1:A:76:THR:CB	0.47	2.62	14	1
1:A:21:TRP:CD2	1:A:58:ILE:HD13	0.47	2.44	2	1
1:A:33:GLU:N	1:A:48:LEU:HD21	0.47	2.23	3	1
1:A:21:TRP:CE3	1:A:36:VAL:HB	0.47	2.45	13	1
1:A:64:ASP:OD2	1:A:65:THR:O	0.47	2.33	9	6
1:A:40:THR:HG22	1:A:41:ASP:N	0.47	2.23	6	2
1:A:3:ASP:CG	1:A:71:LEU:HD11	0.47	2.29	13	1
1:A:22:HIS:NE2	1:A:37:ASP:OD2	0.47	2.47	24	1
1:A:54:VAL:O	1:A:55:ILE:O	0.47	2.33	6	2
1:A:8:THR:HG23	1:A:68:SER:OG	0.46	2.09	4	1
1:A:40:THR:CG2	1:A:43:VAL:HB	0.46	2.40	24	1
1:A:10:PRO:O	1:A:13:ILE:O	0.46	2.33	10	9
1:A:38:ILE:HD11	1:A:47:VAL:CG2	0.46	2.40	9	2
1:A:2:ILE:HD12	1:A:2:ILE:O	0.46	2.09	20	1
1:A:27:GLU:OE1	1:A:28:ALA:O	0.46	2.34	3	2
1:A:29:VAL:O	1:A:52:ASP:OD2	0.46	2.34	20	1
1:A:36:VAL:CG1	1:A:47:VAL:HB	0.46	2.40	8	18
1:A:27:GLU:OE2	1:A:28:ALA:O	0.46	2.34	11	4
1:A:71:LEU:C	1:A:71:LEU:CD2	0.46	2.83	10	1
1:A:60:LYS:CD	1:A:66:VAL:HG12	0.46	2.41	19	1
1:A:35:ILE:HG13	1:A:49:ALA:HB2	0.46	1.87	1	3
1:A:57:GLU:OE2	1:A:74:LYS:NZ	0.46	2.49	1	1
1:A:64:ASP:OD1	1:A:65:THR:O	0.46	2.34	7	6
1:A:34:LEU:HG	1:A:35:ILE:N	0.46	2.26	14	12
1:A:38:ILE:HD13	1:A:38:ILE:N	0.46	2.26	3	1
1:A:17:THR:O	1:A:39:GLU:HG3	0.46	2.11	10	1
1:A:29:VAL:CG2	1:A:30:LYS:N	0.46	2.78	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PRO:HB3	1:A:55:ILE:CG2	0.46	2.41	19	1
1:A:55:ILE:HA	1:A:75:LEU:HD12	0.46	1.88	13	1
1:A:60:LYS:CD	1:A:64:ASP:CG	0.46	2.84	13	1
1:A:60:LYS:HG3	1:A:64:ASP:OD1	0.45	2.11	21	3
1:A:31:ARG:CG	1:A:51:ALA:HA	0.45	2.41	6	1
1:A:52:ASP:OD1	1:A:53:GLY:N	0.45	2.49	12	6
1:A:25:PRO:HD3	1:A:58:ILE:CD1	0.45	2.42	19	2
1:A:11:GLU:O	1:A:12:SER:C	0.45	2.54	2	25
1:A:55:ILE:HG22	1:A:56:ALA:H	0.45	1.69	6	3
1:A:21:TRP:CE2	1:A:58:ILE:HG21	0.45	2.47	11	2
1:A:30:LYS:O	1:A:33:GLU:CB	0.45	2.65	8	1
1:A:2:ILE:HD12	1:A:75:LEU:HD13	0.45	1.87	23	1
1:A:67:LEU:HD23	1:A:68:SER:N	0.45	2.27	21	1
1:A:20:THR:HG23	1:A:62:GLU:OE1	0.45	2.11	23	1
1:A:34:LEU:HA	1:A:48:LEU:HD22	0.45	1.88	23	1
1:A:2:ILE:HD12	1:A:75:LEU:HD22	0.45	1.89	25	1
1:A:38:ILE:CG2	1:A:45:MET:HB2	0.44	2.42	2	3
1:A:4:ILE:HG23	1:A:47:VAL:HG11	0.44	1.89	3	1
1:A:71:LEU:HD21	1:A:74:LYS:HD2	0.44	1.89	3	1
1:A:60:LYS:HA	1:A:60:LYS:CE	0.44	2.42	9	2
1:A:2:ILE:CD1	1:A:75:LEU:HD23	0.44	2.42	13	1
1:A:60:LYS:CD	1:A:70:GLU:HG2	0.44	2.42	24	1
1:A:21:TRP:CE2	1:A:58:ILE:HG23	0.44	2.48	15	1
1:A:36:VAL:O	1:A:47:VAL:HG23	0.44	2.13	25	1
1:A:2:ILE:HD12	1:A:2:ILE:N	0.44	2.27	1	2
1:A:42:LYS:C	1:A:43:VAL:HG23	0.44	2.33	14	2
1:A:15:ASP:OD1	1:A:15:ASP:N	0.44	2.50	9	1
1:A:21:TRP:O	1:A:22:HIS:C	0.44	2.56	11	24
1:A:25:PRO:CB	1:A:57:GLU:HA	0.44	2.43	20	7
1:A:36:VAL:O	1:A:36:VAL:HG13	0.44	2.12	10	3
1:A:39:GLU:HG2	1:A:44:VAL:HG22	0.44	1.89	24	1
1:A:33:GLU:O	1:A:34:LEU:O	0.44	2.36	5	9
1:A:30:LYS:O	1:A:31:ARG:C	0.44	2.56	2	24
1:A:40:THR:O	1:A:41:ASP:C	0.44	2.56	22	25
1:A:71:LEU:HD11	1:A:74:LYS:CG	0.44	2.43	8	1
1:A:16:GLY:O	1:A:65:THR:CG2	0.44	2.66	12	1
1:A:17:THR:O	1:A:18:VAL:O	0.44	2.36	24	6
1:A:32:ASP:HA	1:A:48:LEU:CD2	0.44	2.42	3	1
1:A:20:THR:HA	1:A:62:GLU:CB	0.44	2.42	22	3
1:A:10:PRO:HD2	1:A:13:ILE:HD12	0.44	1.88	8	1
1:A:33:GLU:O	1:A:34:LEU:C	0.44	2.57	1	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LYS:HG2	1:A:64:ASP:OD1	0.43	2.12	12	4
1:A:60:LYS:HD2	1:A:64:ASP:OD2	0.43	2.13	9	2
1:A:31:ARG:O	1:A:32:ASP:HB3	0.43	2.13	11	8
1:A:60:LYS:HG2	1:A:64:ASP:OD2	0.43	2.12	5	2
1:A:34:LEU:HA	1:A:48:LEU:CD1	0.43	2.43	12	1
1:A:19:ALA:CB	1:A:37:ASP:HB3	0.43	2.43	17	2
1:A:54:VAL:H	1:A:76:THR:HG22	0.43	1.73	24	1
1:A:31:ARG:HG2	1:A:51:ALA:N	0.43	2.29	6	1
1:A:7:PRO:HG2	1:A:9:PHE:CZ	0.43	2.48	10	1
1:A:33:GLU:C	1:A:48:LEU:HD12	0.43	2.33	20	1
1:A:18:VAL:CG1	1:A:62:GLU:HA	0.43	2.44	13	9
1:A:17:THR:O	1:A:18:VAL:C	0.43	2.57	21	7
1:A:17:THR:O	1:A:39:GLU:HB2	0.43	2.13	1	3
1:A:8:THR:O	1:A:9:PHE:CD1	0.43	2.72	2	1
1:A:25:PRO:CG	1:A:57:GLU:HA	0.43	2.44	17	4
1:A:25:PRO:HA	1:A:55:ILE:CG2	0.43	2.43	11	1
1:A:17:THR:O	1:A:39:GLU:HG2	0.43	2.13	7	1
1:A:17:THR:O	1:A:39:GLU:HB3	0.43	2.14	15	1
1:A:2:ILE:HD13	1:A:75:LEU:HD22	0.43	1.89	1	1
1:A:13:ILE:CG1	1:A:41:ASP:OD1	0.43	2.66	13	1
1:A:48:LEU:HG	1:A:49:ALA:N	0.43	2.29	20	1
1:A:66:VAL:HG23	1:A:67:LEU:N	0.43	2.28	2	1
1:A:21:TRP:CE2	1:A:58:ILE:CG2	0.43	3.02	15	1
1:A:24:LYS:CB	1:A:25:PRO:HD2	0.42	2.44	2	1
1:A:67:LEU:O	1:A:70:GLU:HB2	0.42	2.15	14	2
1:A:3:ASP:OD2	1:A:5:LYS:HG3	0.42	2.14	15	1
1:A:40:THR:HG21	1:A:45:MET:SD	0.42	2.54	4	1
1:A:9:PHE:CD2	1:A:68:SER:HB2	0.42	2.49	16	1
1:A:25:PRO:HB3	1:A:55:ILE:HG22	0.42	1.91	19	1
1:A:40:THR:HG22	1:A:41:ASP:H	0.42	1.74	16	2
1:A:3:ASP:OD2	1:A:71:LEU:HD11	0.42	2.15	18	2
1:A:7:PRO:O	1:A:8:THR:C	0.42	2.58	4	1
1:A:22:HIS:CE1	1:A:34:LEU:HG	0.42	2.50	12	2
1:A:19:ALA:HB3	1:A:37:ASP:HB3	0.42	1.91	17	1
1:A:9:PHE:CE2	1:A:15:ASP:CA	0.42	3.02	22	1
1:A:24:LYS:HD2	1:A:25:PRO:CD	0.42	2.44	25	1
1:A:27:GLU:CD	1:A:28:ALA:O	0.42	2.58	3	4
1:A:8:THR:O	1:A:9:PHE:C	0.42	2.57	5	1
1:A:36:VAL:O	1:A:47:VAL:HB	0.42	2.15	20	5
1:A:31:ARG:HG2	1:A:32:ASP:N	0.42	2.29	20	1
1:A:66:VAL:C	1:A:67:LEU:HD23	0.42	2.34	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:CD1	1:A:48:LEU:HD12	0.42	2.44	15	1
1:A:29:VAL:HG21	1:A:35:ILE:CD1	0.42	2.42	5	1
1:A:55:ILE:H	1:A:55:ILE:HD12	0.42	1.75	6	1
1:A:60:LYS:NZ	1:A:72:LEU:HD23	0.42	2.30	6	1
1:A:25:PRO:CA	1:A:55:ILE:HB	0.42	2.45	10	1
1:A:58:ILE:HG22	1:A:60:LYS:O	0.41	2.16	6	2
1:A:34:LEU:CD1	1:A:46:GLU:HB3	0.41	2.45	10	1
1:A:71:LEU:HD21	1:A:74:LYS:HD3	0.41	1.91	13	1
1:A:35:ILE:CG1	1:A:49:ALA:HB2	0.41	2.45	14	1
1:A:70:GLU:OE2	1:A:72:LEU:CD2	0.41	2.69	9	1
1:A:71:LEU:HD21	1:A:74:LYS:CG	0.41	2.45	13	1
1:A:34:LEU:N	1:A:48:LEU:HG	0.41	2.29	15	2
1:A:33:GLU:C	1:A:48:LEU:HD13	0.41	2.35	23	1
1:A:3:ASP:OD1	1:A:3:ASP:C	0.41	2.59	1	1
1:A:21:TRP:CD2	1:A:58:ILE:CD1	0.41	3.04	2	1
1:A:13:ILE:HG12	1:A:41:ASP:OD1	0.41	2.14	13	1
1:A:12:SER:O	1:A:12:SER:OG	0.41	2.33	2	1
1:A:33:GLU:O	1:A:48:LEU:HD12	0.41	2.16	20	1
1:A:60:LYS:HE2	1:A:70:GLU:CG	0.41	2.45	6	1
1:A:31:ARG:CD	1:A:32:ASP:N	0.41	2.84	17	1
1:A:54:VAL:O	1:A:76:THR:HB	0.41	2.16	24	1
1:A:51:ALA:O	1:A:52:ASP:O	0.41	2.39	8	1
1:A:44:VAL:O	1:A:44:VAL:CG1	0.41	2.68	13	1
1:A:36:VAL:O	1:A:47:VAL:CG2	0.41	2.68	25	1
1:A:14:ALA:C	1:A:15:ASP:OD1	0.41	2.59	1	1
1:A:11:GLU:O	1:A:13:ILE:HG12	0.41	2.16	2	1
1:A:24:LYS:CB	1:A:25:PRO:CD	0.41	2.99	2	1
1:A:38:ILE:CG1	1:A:47:VAL:CG2	0.41	2.99	9	1
1:A:19:ALA:O	1:A:62:GLU:OE1	0.41	2.39	10	1
1:A:60:LYS:HG3	1:A:64:ASP:OD2	0.41	2.16	11	1
1:A:18:VAL:HG11	1:A:62:GLU:HA	0.41	1.93	13	1
1:A:40:THR:CG2	1:A:41:ASP:N	0.41	2.79	18	1
1:A:40:THR:HB	1:A:43:VAL:O	0.41	2.16	6	1
1:A:38:ILE:HG13	1:A:47:VAL:CG2	0.41	2.46	16	1
1:A:3:ASP:OD2	1:A:5:LYS:CE	0.40	2.68	1	1
1:A:38:ILE:HD11	1:A:47:VAL:HG23	0.40	1.92	6	1
1:A:44:VAL:O	1:A:44:VAL:HG13	0.40	2.16	12	1
1:A:36:VAL:HG13	1:A:47:VAL:CG2	0.40	2.45	20	1
1:A:36:VAL:HG13	1:A:47:VAL:HG21	0.40	1.94	20	1
1:A:11:GLU:HB2	1:A:13:ILE:CG1	0.40	2.47	2	1
1:A:39:GLU:OE2	1:A:40:THR:O	0.40	2.39	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ILE:CD1	1:A:41:ASP:HB2	0.40	2.46	14	1
1:A:36:VAL:HG13	1:A:36:VAL:O	0.40	2.16	2	1
1:A:2:ILE:O	1:A:2:ILE:HG22	0.40	2.17	13	1
1:A:36:VAL:HG13	1:A:47:VAL:HB	0.40	1.93	23	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	75/79 (95%)	57±3 (76±3%)	15±3 (20±4%)	3±1 (4±2%)	6	34
All	All	1875/1975 (95%)	1426 (76%)	381 (20%)	68 (4%)	6	34

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	18	VAL	17
1	A	34	LEU	15
1	A	51	ALA	14
1	A	15	ASP	12
1	A	52	ASP	3
1	A	55	ILE	2
1	A	35	ILE	2
1	A	31	ARG	1
1	A	57	GLU	1
1	A	26	GLY	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	62/63 (98%)	48±2 (77±3%)	14±2 (23±3%)	3 29
All	All	1550/1575 (98%)	1196 (77%)	354 (23%)	3 29

All 33 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	52	ASP	25
1	A	64	ASP	25
1	A	15	ASP	24
1	A	48	LEU	21
1	A	60	LYS	20
1	A	50	GLU	19
1	A	67	LEU	19
1	A	23	LYS	16
1	A	24	LYS	15
1	A	40	THR	13
1	A	62	GLU	13
1	A	57	GLU	12
1	A	75	LEU	11
1	A	5	LYS	11
1	A	30	LYS	10
1	A	39	GLU	10
1	A	31	ARG	10
1	A	46	GLU	9
1	A	8	THR	9
1	A	74	LYS	8
1	A	11	GLU	8
1	A	71	LEU	7
1	A	12	SER	6
1	A	45	MET	6
1	A	68	SER	4
1	A	33	GLU	4
1	A	72	LEU	4
1	A	42	LYS	4
1	A	27	GLU	3
1	A	17	THR	3
1	A	41	ASP	2
1	A	70	GLU	2
1	A	29	VAL	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