



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 AM UTC

PDB ID : 1FGP / pdb_00001fgp
Title : MEMBRANE PENETRATION DOMAIN OF THE MINOR COAT PROTEIN G3P OF PHAGE FD, NMR, 15 STRUCTURES
Authors : Holliger, P.; Riechmann, L.
Deposited on : 1996-12-10

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

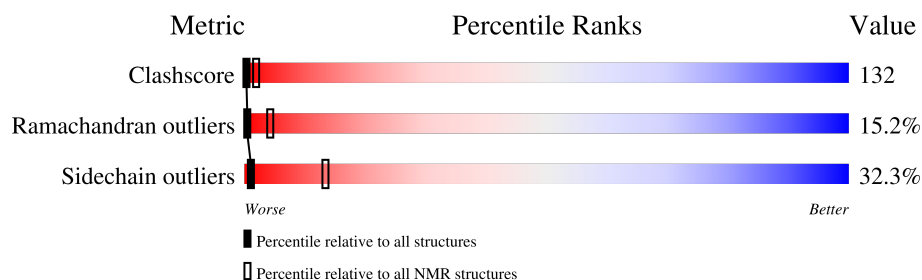
1 Overall quality at a glance

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	A	70	

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 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:3-A:65 (63)	0.52	1

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 and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 11, 12
2	5, 9, 10, 13
Single-model clusters	8; 14; 15

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1038 atoms, of which 497 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FD GENE 3 PROTEIN.

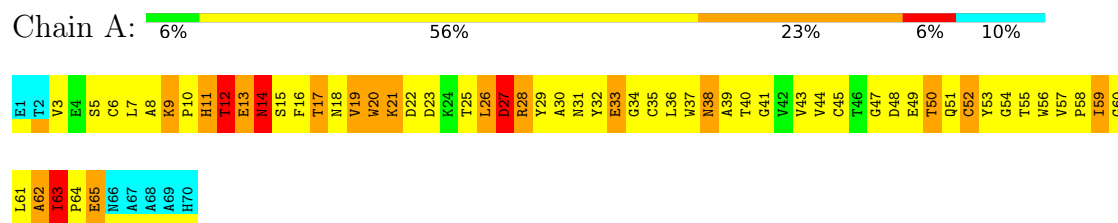
Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1038	338	497	89	110	4	

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: FD GENE 3 PROTEIN

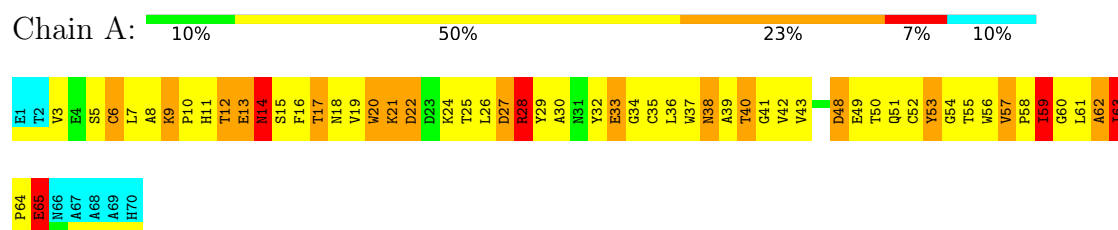


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

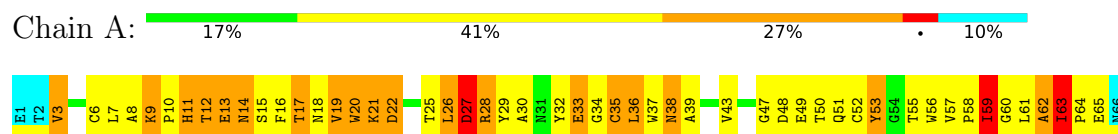
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: FD GENE 3 PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: FD GENE 3 PROTEIN



A67
A68
A69
H70

4.2.3 Score per residue for model 3

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 11% 51% 21% 6% 10%

E1 T2 V3 E4 E5 C6 L7 A8 K9 P10 H11 H12 E13 E14 S15 F16 F17 T17 N18 V19 W20 K21 D22 T25 L26 D27 R28 Y29 A30 N31 Y32 E33 G34 C35 L36 W37 N38 A39 V43 V44 G47 D48 E49 T50 Q51 C52 Y53 G54 T55 W56 V57 P58 I59 G60 L61 A62 I63 P64

E65 N66 A67 A68 A69 H70

4.2.4 Score per residue for model 4

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 11% 46% 29% • 10%

E1 T2 V3 C6 L7 A8 K9 P10 H11 H12 E13 E14 S15 F16 F17 T17 N18 V19 W20 K21 D22 T25 L26 D27 R28 Y29 A30 N31 Y32 E33 G34 C35 L36 W37 N38 A39 T40 G41 V42 V43 V44 G47 D48 E49 T50 Q51 C52 Y53 G54 T55 W56 V57 P58 I59 G60 L61 A62 I63

P64 E65 N66 A67 A68 A69 H70

4.2.5 Score per residue for model 5

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 10% 49% 26% 6% 10%

E1 T2 V3 E4 E5 C6 L7 A8 K9 P10 H11 H12 E13 E14 S15 F16 F17 T17 N18 V19 W20 K21 D22 D23 K24 T25 L26 D27 R28 Y29 A30 N31 Y32 E33 G34 C35 L36 W37 N38 A39 T40 V43 V44 G47 D48 E49 T50 Q51 C52 Y53 G54 T55 W56 V57 P58 I59 G60 L61 A62

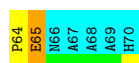
I63 P64 E65 N66 A67 A68 A69 H70

4.2.6 Score per residue for model 6

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 13% 47% 23% 7% 10%

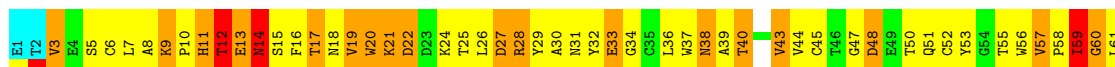
E1 T2 V3 E4 E5 C6 L7 A8 K9 P10 H11 H12 E13 E14 S15 F16 F17 T17 N18 V19 W20 K21 D22 T25 L26 D27 R28 Y29 A30 N31 G34 C35 L36 W37 N38 A39 V42 V43 V44 C45 T46 G47 D48 E49 T50 Q51 C52 Y53 G54 T55 W56 V57 P58 I59 G60 L61 A62 I63



4.2.7 Score per residue for model 7

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 11% 44% 29% 6% 10%



4.2.8 Score per residue for model 8

- Molecule 1: FD GENE 3 PROTEIN

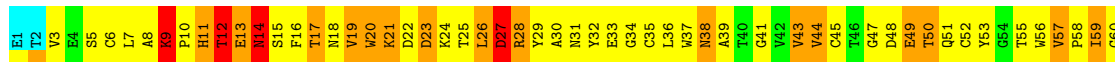
Chain A: 14% 43% 24% 9% 10%



4.2.9 Score per residue for model 9

- Molecule 1: FD GENE 3 PROTEIN

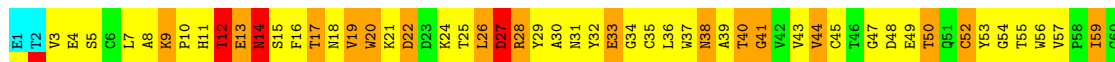
Chain A: 7% 50% 26% 7% 10%



4.2.10 Score per residue for model 10

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 10% 50% 24% 6% 10%

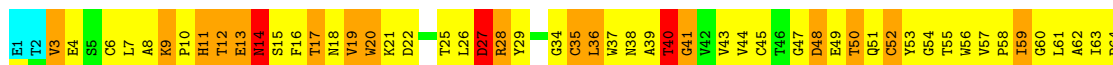




4.2.11 Score per residue for model 11

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 13% 50% 23% • 10%



4.2.12 Score per residue for model 12

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 10% 41% 29% 10% 10%



4.2.13 Score per residue for model 13

- Molecule 1: FD GENE 3 PROTEIN

Chain A: 6% 53% 27% • 10%

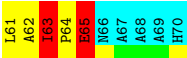


4.2.14 Score per residue for model 14

- Molecule 1: FD GENE 3 PROTEIN

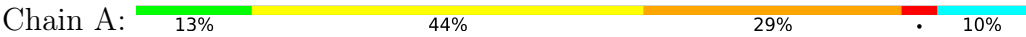
Chain A: 9% 56% 16% 10% 10%





4.2.15 Score per residue for model 15

● Molecule 1: FD GENE 3 PROTEIN



5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *LOWEST TOTAL ENERGIES*.

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

Software name	Classification	Version
X-PLOR	refinement	
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.38±0.01	0±0/505 (0.0± 0.0%)	1.31±0.02	0±1/694 (0.0± 0.1%)
All	All	1.38	1/7575 (0.0%)	1.31	5/10410 (0.0%)

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±0.0
All	All	0	15

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	60	GLY	N-CA	5.66	1.49	1.44	7	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	ILE	CA-C-N	-5.56	117.88	122.16	6	1
1	A	59	ILE	C-N-CA	-5.56	117.88	122.16	6	1
1	A	23	ASP	N-CA-C	-5.46	106.57	113.18	12	2
1	A	8	ALA	N-CA-C	-5.11	106.89	113.02	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	28	ARG	Sidechain	15

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	A	491	454	454	124±11
All	All	7365	6810	6810	1864

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 131.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ASN:HA	1:A:36:LEU:HD12	0.86	1.47	15	1
1:A:3:VAL:HG22	1:A:61:LEU:HD21	0.85	1.46	3	5
1:A:39:ALA:HB2	1:A:56:TRP:CE3	0.82	2.08	6	10
1:A:12:THR:HG23	1:A:55:THR:HG22	0.82	1.51	12	15
1:A:36:LEU:HD13	1:A:59:ILE:HD11	0.82	1.51	6	3
1:A:28:ARG:HB3	1:A:39:ALA:HB3	0.81	1.52	4	13
1:A:29:TYR:HB3	1:A:36:LEU:HD11	0.81	1.50	1	5
1:A:38:ASN:HB3	1:A:59:ILE:HD12	0.81	1.50	6	7
1:A:16:PHE:HB3	1:A:30:ALA:HB1	0.80	1.52	15	14
1:A:16:PHE:CB	1:A:30:ALA:HB1	0.80	2.07	10	13
1:A:20:TRP:CZ3	1:A:36:LEU:HD21	0.80	2.12	12	3
1:A:59:ILE:N	1:A:59:ILE:HD13	0.78	1.93	10	14
1:A:3:VAL:HG12	1:A:7:LEU:CD1	0.78	2.08	13	8
1:A:39:ALA:HB2	1:A:56:TRP:CZ3	0.77	2.15	2	5
1:A:3:VAL:HG12	1:A:7:LEU:HD11	0.77	1.55	8	7
1:A:19:VAL:HG21	1:A:56:TRP:CH2	0.76	2.15	11	12
1:A:36:LEU:CD1	1:A:59:ILE:HD11	0.76	2.09	6	3
1:A:3:VAL:HG22	1:A:7:LEU:CD1	0.75	2.11	10	3
1:A:3:VAL:HB	1:A:61:LEU:HD21	0.75	1.54	14	2
1:A:39:ALA:HB1	1:A:43:VAL:HG21	0.75	1.58	8	8
1:A:7:LEU:HD21	1:A:59:ILE:HA	0.75	1.56	7	4
1:A:44:VAL:O	1:A:44:VAL:HG23	0.75	1.80	3	1
1:A:20:TRP:CH2	1:A:36:LEU:HD11	0.73	2.19	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TRP:CH2	1:A:36:LEU:HD21	0.72	2.19	5	3
1:A:36:LEU:C	1:A:36:LEU:HD13	0.72	2.08	2	3
1:A:20:TRP:CZ2	1:A:63:ILE:HD13	0.72	2.19	10	14
1:A:63:ILE:N	1:A:64:PRO:CD	0.72	2.52	14	14
1:A:12:THR:OG1	1:A:56:TRP:N	0.72	2.23	14	15
1:A:12:THR:CG2	1:A:55:THR:HG22	0.72	2.14	15	9
1:A:42:VAL:O	1:A:42:VAL:HG13	0.71	1.84	12	1
1:A:36:LEU:HD22	1:A:63:ILE:H	0.71	1.44	8	7
1:A:50:THR:HG23	1:A:51:GLN:HG3	0.70	1.64	15	2
1:A:36:LEU:HD13	1:A:36:LEU:O	0.70	1.86	2	1
1:A:9:LYS:HB3	1:A:10:PRO:HD2	0.70	1.62	11	15
1:A:44:VAL:HG13	1:A:44:VAL:O	0.70	1.87	8	2
1:A:20:TRP:CD1	1:A:21:LYS:N	0.69	2.60	4	15
1:A:63:ILE:O	1:A:63:ILE:HG23	0.69	1.86	6	2
1:A:16:PHE:CD2	1:A:30:ALA:HB1	0.69	2.22	13	4
1:A:29:TYR:CD1	1:A:36:LEU:HD11	0.69	2.23	6	4
1:A:36:LEU:HD22	1:A:63:ILE:N	0.69	2.03	8	7
1:A:36:LEU:HD23	1:A:64:PRO:O	0.69	1.88	7	6
1:A:43:VAL:HG12	1:A:53:TYR:O	0.68	1.87	3	4
1:A:38:ASN:CB	1:A:59:ILE:HD12	0.68	2.18	10	8
1:A:20:TRP:CZ3	1:A:36:LEU:HD11	0.67	2.25	4	6
1:A:16:PHE:O	1:A:19:VAL:HG23	0.67	1.90	6	4
1:A:38:ASN:HB2	1:A:59:ILE:HD11	0.66	1.67	3	2
1:A:38:ASN:HB3	1:A:59:ILE:HD11	0.66	1.67	8	2
1:A:50:THR:HG23	1:A:51:GLN:CG	0.66	2.20	1	1
1:A:29:TYR:CZ	1:A:65:GLU:CG	0.66	2.78	13	1
1:A:27:ASP:CB	1:A:29:TYR:CE2	0.66	2.79	11	6
1:A:36:LEU:HD13	1:A:63:ILE:N	0.65	2.06	3	5
1:A:59:ILE:HD13	1:A:59:ILE:H	0.65	1.49	9	5
1:A:16:PHE:CD2	1:A:17:THR:O	0.65	2.50	15	4
1:A:39:ALA:HB2	1:A:56:TRP:CD2	0.65	2.26	6	1
1:A:20:TRP:CZ2	1:A:63:ILE:CD1	0.64	2.81	14	4
1:A:22:ASP:N	1:A:22:ASP:OD1	0.64	2.27	12	1
1:A:29:TYR:CE2	1:A:38:ASN:CB	0.64	2.80	12	1
1:A:20:TRP:CH2	1:A:63:ILE:HD13	0.64	2.28	8	4
1:A:61:LEU:O	1:A:62:ALA:HB2	0.64	1.90	7	11
1:A:43:VAL:HG12	1:A:52:CYS:SG	0.63	2.33	10	5
1:A:36:LEU:HD23	1:A:62:ALA:HA	0.63	1.71	5	3
1:A:53:TYR:CG	1:A:54:GLY:N	0.63	2.66	1	9
1:A:9:LYS:CD	1:A:37:TRP:CZ2	0.63	2.81	8	5
1:A:20:TRP:CH2	1:A:29:TYR:CB	0.63	2.82	1	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:VAL:O	1:A:7:LEU:HD12	0.62	1.94	11	2
1:A:3:VAL:CG2	1:A:61:LEU:HD21	0.62	2.21	3	2
1:A:16:PHE:CZ	1:A:17:THR:O	0.62	2.53	3	6
1:A:29:TYR:CD2	1:A:36:LEU:CD2	0.62	2.83	15	1
1:A:16:PHE:CE2	1:A:17:THR:O	0.62	2.53	2	10
1:A:36:LEU:HD12	1:A:59:ILE:HG12	0.62	1.71	2	1
1:A:53:TYR:CD1	1:A:54:GLY:N	0.61	2.67	4	5
1:A:56:TRP:N	1:A:56:TRP:CD1	0.61	2.68	12	13
1:A:27:ASP:CB	1:A:29:TYR:CE1	0.61	2.82	13	6
1:A:28:ARG:CB	1:A:39:ALA:HB3	0.61	2.25	3	11
1:A:16:PHE:CD1	1:A:17:THR:O	0.60	2.54	1	5
1:A:37:TRP:HB3	1:A:56:TRP:CB	0.60	2.25	10	15
1:A:3:VAL:CG1	1:A:7:LEU:CD1	0.60	2.79	6	2
1:A:29:TYR:CE1	1:A:38:ASN:CB	0.60	2.84	8	2
1:A:36:LEU:HD23	1:A:62:ALA:O	0.60	1.97	14	3
1:A:62:ALA:O	1:A:63:ILE:CB	0.60	2.49	13	11
1:A:43:VAL:HG13	1:A:53:TYR:O	0.60	1.97	4	4
1:A:26:LEU:O	1:A:27:ASP:CB	0.60	2.49	13	15
1:A:20:TRP:HZ3	1:A:36:LEU:HD21	0.59	1.56	12	2
1:A:25:THR:OG1	1:A:29:TYR:CE2	0.59	2.55	11	8
1:A:27:ASP:O	1:A:29:TYR:CE2	0.59	2.55	10	3
1:A:44:VAL:O	1:A:44:VAL:CG1	0.59	2.49	11	2
1:A:20:TRP:CE2	1:A:22:ASP:OD1	0.59	2.55	12	1
1:A:3:VAL:CB	1:A:61:LEU:HD21	0.59	2.26	14	1
1:A:11:HIS:O	1:A:12:THR:CB	0.59	2.51	8	8
1:A:63:ILE:N	1:A:64:PRO:HD3	0.59	2.11	6	4
1:A:43:VAL:HG11	1:A:56:TRP:CZ2	0.59	2.31	15	5
1:A:28:ARG:C	1:A:29:TYR:CD1	0.59	2.80	12	6
1:A:16:PHE:CE1	1:A:17:THR:O	0.59	2.56	1	5
1:A:29:TYR:HB3	1:A:36:LEU:HD21	0.59	1.74	2	3
1:A:28:ARG:HB2	1:A:39:ALA:HB3	0.59	1.74	8	1
1:A:59:ILE:N	1:A:59:ILE:CD1	0.59	2.66	10	10
1:A:12:THR:CG2	1:A:13:GLU:N	0.59	2.65	1	15
1:A:12:THR:CG2	1:A:55:THR:CG2	0.58	2.81	11	9
1:A:27:ASP:O	1:A:29:TYR:CD2	0.58	2.56	7	6
1:A:36:LEU:HD13	1:A:37:TRP:N	0.58	2.14	12	3
1:A:25:THR:OG1	1:A:29:TYR:CE1	0.58	2.55	15	3
1:A:20:TRP:HZ3	1:A:36:LEU:HD11	0.58	1.58	15	1
1:A:37:TRP:HB3	1:A:56:TRP:HB3	0.58	1.75	9	15
1:A:19:VAL:HG11	1:A:56:TRP:CZ3	0.58	2.33	9	2
1:A:3:VAL:HG22	1:A:7:LEU:HD11	0.58	1.76	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:THR:HG23	1:A:55:THR:CG2	0.58	2.27	15	9
1:A:12:THR:OG1	1:A:57:VAL:N	0.57	2.37	1	15
1:A:29:TYR:OH	1:A:65:GLU:CG	0.57	2.52	12	1
1:A:9:LYS:CB	1:A:9:LYS:NZ	0.57	2.67	14	1
1:A:20:TRP:CZ3	1:A:29:TYR:HB2	0.57	2.34	15	4
1:A:32:TYR:O	1:A:33:GLU:C	0.57	2.47	5	13
1:A:7:LEU:HD21	1:A:59:ILE:CA	0.57	2.29	7	4
1:A:37:TRP:N	1:A:37:TRP:CD1	0.57	2.72	12	3
1:A:29:TYR:CE2	1:A:38:ASN:HB3	0.57	2.34	12	1
1:A:8:ALA:O	1:A:9:LYS:O	0.57	2.23	6	14
1:A:9:LYS:HD3	1:A:37:TRP:CZ2	0.57	2.33	8	14
1:A:25:THR:O	1:A:26:LEU:CB	0.57	2.52	13	11
1:A:12:THR:HA	1:A:56:TRP:C	0.57	2.24	9	15
1:A:32:TYR:CD2	1:A:32:TYR:O	0.57	2.57	3	1
1:A:27:ASP:HB3	1:A:29:TYR:CE1	0.57	2.35	13	6
1:A:3:VAL:CG1	1:A:7:LEU:HD11	0.57	2.30	13	3
1:A:9:LYS:CE	1:A:37:TRP:CZ2	0.56	2.88	2	6
1:A:29:TYR:CE1	1:A:65:GLU:HG2	0.56	2.35	13	1
1:A:9:LYS:CB	1:A:10:PRO:CD	0.56	2.83	14	8
1:A:63:ILE:HG22	1:A:63:ILE:O	0.56	2.00	15	1
1:A:63:ILE:O	1:A:63:ILE:CG2	0.56	2.54	14	2
1:A:19:VAL:HG21	1:A:56:TRP:HH2	0.56	1.60	11	6
1:A:16:PHE:CZ	1:A:31:ASN:O	0.56	2.58	10	1
1:A:20:TRP:CH2	1:A:29:TYR:HB2	0.56	2.36	1	7
1:A:53:TYR:CD1	1:A:53:TYR:C	0.56	2.84	3	3
1:A:20:TRP:CZ3	1:A:29:TYR:CB	0.56	2.89	10	4
1:A:44:VAL:O	1:A:44:VAL:CG2	0.56	2.54	3	1
1:A:7:LEU:HD23	1:A:58:PRO:O	0.56	2.00	11	1
1:A:36:LEU:HD22	1:A:37:TRP:N	0.56	2.16	2	3
1:A:12:THR:O	1:A:14:ASN:N	0.55	2.40	13	15
1:A:19:VAL:HG13	1:A:29:TYR:O	0.55	2.01	9	4
1:A:20:TRP:NE1	1:A:22:ASP:OD1	0.55	2.40	12	1
1:A:29:TYR:CE2	1:A:65:GLU:HG3	0.55	2.36	13	1
1:A:64:PRO:O	1:A:65:GLU:CB	0.55	2.54	15	1
1:A:57:VAL:O	1:A:59:ILE:HD13	0.55	2.00	11	3
1:A:32:TYR:O	1:A:32:TYR:CG	0.55	2.60	3	4
1:A:29:TYR:CZ	1:A:65:GLU:HG3	0.55	2.34	13	1
1:A:20:TRP:CH2	1:A:29:TYR:HB3	0.55	2.37	5	6
1:A:20:TRP:CG	1:A:21:LYS:N	0.55	2.74	15	11
1:A:63:ILE:N	1:A:64:PRO:HD2	0.55	2.16	9	10
1:A:25:THR:HG21	1:A:63:ILE:O	0.55	2.02	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ARG:HG2	1:A:39:ALA:HB3	0.55	1.78	15	2
1:A:12:THR:OG1	1:A:55:THR:C	0.55	2.49	15	15
1:A:31:ASN:CA	1:A:36:LEU:HD12	0.55	2.28	15	1
1:A:59:ILE:H	1:A:59:ILE:HD13	0.55	1.62	15	1
1:A:36:LEU:CD1	1:A:59:ILE:CG1	0.55	2.84	11	2
1:A:3:VAL:HG13	1:A:60:GLY:HA2	0.55	1.77	11	1
1:A:19:VAL:HG11	1:A:56:TRP:HZ3	0.55	1.63	3	2
1:A:29:TYR:CE2	1:A:38:ASN:HB2	0.55	2.37	13	4
1:A:36:LEU:CG	1:A:62:ALA:O	0.55	2.55	6	3
1:A:29:TYR:CD2	1:A:36:LEU:HD21	0.55	2.37	15	1
1:A:9:LYS:CB	1:A:10:PRO:HD2	0.54	2.31	14	8
1:A:43:VAL:CG1	1:A:53:TYR:O	0.54	2.55	3	7
1:A:25:THR:O	1:A:26:LEU:HB2	0.54	2.02	12	8
1:A:15:SER:CB	1:A:53:TYR:HA	0.54	2.33	11	15
1:A:27:ASP:C	1:A:29:TYR:CE1	0.54	2.86	12	4
1:A:9:LYS:HB3	1:A:10:PRO:CD	0.54	2.32	11	14
1:A:38:ASN:CB	1:A:59:ILE:CD1	0.54	2.85	13	3
1:A:19:VAL:N	1:A:50:THR:O	0.54	2.39	9	4
1:A:19:VAL:HG12	1:A:20:TRP:N	0.54	2.16	11	5
1:A:47:GLY:O	1:A:50:THR:HG22	0.54	2.02	7	1
1:A:22:ASP:CB	1:A:25:THR:OG1	0.54	2.55	2	4
1:A:11:HIS:O	1:A:12:THR:C	0.54	2.51	6	7
1:A:27:ASP:HB3	1:A:29:TYR:CZ	0.54	2.38	1	5
1:A:65:GLU:N	1:A:65:GLU:OE1	0.54	2.41	13	1
1:A:37:TRP:CD1	1:A:37:TRP:N	0.54	2.76	6	12
1:A:36:LEU:HD13	1:A:37:TRP:O	0.54	2.03	1	3
1:A:61:LEU:O	1:A:62:ALA:CB	0.54	2.56	7	7
1:A:23:ASP:O	1:A:26:LEU:CD2	0.54	2.56	14	2
1:A:22:ASP:OD2	1:A:25:THR:HG21	0.54	2.03	12	1
1:A:57:VAL:O	1:A:59:ILE:CD1	0.53	2.56	11	5
1:A:63:ILE:H	1:A:64:PRO:HD2	0.53	1.63	1	9
1:A:27:ASP:HB3	1:A:29:TYR:CE2	0.53	2.37	11	4
1:A:36:LEU:CD2	1:A:62:ALA:O	0.53	2.56	14	3
1:A:36:LEU:HD22	1:A:64:PRO:CD	0.53	2.33	15	1
1:A:11:HIS:O	1:A:13:GLU:N	0.53	2.42	6	7
1:A:38:ASN:ND2	1:A:38:ASN:C	0.53	2.66	10	11
1:A:3:VAL:O	1:A:7:LEU:CD1	0.53	2.56	11	2
1:A:37:TRP:CB	1:A:56:TRP:HB3	0.53	2.33	2	15
1:A:36:LEU:CD2	1:A:64:PRO:O	0.53	2.57	3	4
1:A:38:ASN:O	1:A:38:ASN:ND2	0.53	2.42	7	2
1:A:36:LEU:HD22	1:A:63:ILE:C	0.53	2.29	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:TYR:CE1	1:A:38:ASN:HB2	0.53	2.39	8	6
1:A:42:VAL:O	1:A:43:VAL:HG23	0.53	2.03	8	1
1:A:28:ARG:O	1:A:29:TYR:CD1	0.53	2.62	10	3
1:A:20:TRP:CZ2	1:A:29:TYR:HB2	0.53	2.39	14	3
1:A:56:TRP:O	1:A:57:VAL:C	0.53	2.52	11	15
1:A:29:TYR:CE1	1:A:38:ASN:HB3	0.53	2.38	11	2
1:A:45:CYS:SG	1:A:49:GLU:C	0.53	2.92	8	1
1:A:17:THR:O	1:A:18:ASN:CB	0.52	2.57	4	11
1:A:45:CYS:HB3	1:A:49:GLU:HA	0.52	1.80	11	5
1:A:20:TRP:CH2	1:A:63:ILE:HG12	0.52	2.40	15	1
1:A:25:THR:HB	1:A:65:GLU:CG	0.52	2.34	13	1
1:A:35:CYS:N	1:A:61:LEU:O	0.52	2.42	6	3
1:A:7:LEU:CD2	1:A:58:PRO:O	0.52	2.57	9	3
1:A:38:ASN:HB2	1:A:59:ILE:CD1	0.52	2.35	13	3
1:A:41:GLY:O	1:A:43:VAL:N	0.52	2.42	1	1
1:A:48:ASP:O	1:A:49:GLU:CB	0.52	2.57	2	9
1:A:36:LEU:HB2	1:A:62:ALA:CA	0.52	2.35	14	12
1:A:12:THR:O	1:A:13:GLU:C	0.52	2.50	12	15
1:A:59:ILE:HD13	1:A:59:ILE:N	0.52	2.20	15	1
1:A:25:THR:HB	1:A:65:GLU:CD	0.52	2.30	13	1
1:A:41:GLY:O	1:A:43:VAL:CG2	0.52	2.58	9	1
1:A:16:PHE:CD2	1:A:17:THR:N	0.52	2.78	10	1
1:A:16:PHE:CG	1:A:30:ALA:HB1	0.52	2.39	13	3
1:A:9:LYS:HD3	1:A:37:TRP:CH2	0.52	2.39	8	7
1:A:36:LEU:CD1	1:A:59:ILE:HG12	0.52	2.35	11	2
1:A:43:VAL:CG1	1:A:52:CYS:SG	0.52	2.98	7	4
1:A:16:PHE:O	1:A:19:VAL:CG2	0.52	2.58	11	2
1:A:15:SER:HB3	1:A:53:TYR:CD2	0.51	2.40	12	3
1:A:40:THR:HG23	1:A:41:GLY:N	0.51	2.21	13	1
1:A:17:THR:OG1	1:A:18:ASN:N	0.51	2.43	2	3
1:A:35:CYS:CA	1:A:61:LEU:O	0.51	2.58	14	3
1:A:27:ASP:O	1:A:29:TYR:CD1	0.51	2.63	15	3
1:A:36:LEU:C	1:A:36:LEU:CD1	0.51	2.80	2	3
1:A:38:ASN:CB	1:A:59:ILE:HD11	0.51	2.35	3	1
1:A:16:PHE:CE1	1:A:31:ASN:O	0.51	2.64	10	1
1:A:22:ASP:OD2	1:A:29:TYR:CD1	0.51	2.62	12	1
1:A:34:GLY:C	1:A:61:LEU:O	0.51	2.54	7	11
1:A:16:PHE:CE2	1:A:31:ASN:OD1	0.51	2.63	6	1
1:A:39:ALA:CB	1:A:56:TRP:CE3	0.51	2.91	6	1
1:A:44:VAL:C	1:A:52:CYS:SG	0.51	2.94	3	5
1:A:50:THR:HG23	1:A:51:GLN:HG2	0.51	1.81	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:THR:CG2	1:A:55:THR:CB	0.51	2.89	4	7
1:A:29:TYR:CZ	1:A:65:GLU:HG2	0.51	2.40	13	1
1:A:11:HIS:O	1:A:12:THR:HB	0.50	2.05	8	8
1:A:31:ASN:O	1:A:31:ASN:CG	0.50	2.54	15	3
1:A:12:THR:OG1	1:A:55:THR:HB	0.50	2.06	14	8
1:A:9:LYS:HD2	1:A:37:TRP:CZ2	0.50	2.41	14	2
1:A:22:ASP:OD2	1:A:25:THR:CG2	0.50	2.59	12	1
1:A:36:LEU:HB2	1:A:62:ALA:N	0.50	2.21	2	14
1:A:31:ASN:ND2	1:A:31:ASN:O	0.50	2.44	13	1
1:A:36:LEU:CD2	1:A:64:PRO:HD2	0.50	2.37	15	1
1:A:29:TYR:CE1	1:A:38:ASN:OD1	0.50	2.65	1	1
1:A:38:ASN:O	1:A:56:TRP:HA	0.50	2.06	9	15
1:A:62:ALA:O	1:A:63:ILE:HB	0.50	2.05	13	11
1:A:47:GLY:O	1:A:50:THR:OG1	0.50	2.29	13	9
1:A:11:HIS:O	1:A:12:THR:HG22	0.50	2.07	1	8
1:A:16:PHE:CD1	1:A:17:THR:N	0.50	2.79	7	4
1:A:42:VAL:HG12	1:A:42:VAL:O	0.50	2.06	6	1
1:A:9:LYS:HB3	1:A:9:LYS:NZ	0.50	2.22	14	1
1:A:36:LEU:HD13	1:A:59:ILE:HG12	0.50	1.83	11	1
1:A:28:ARG:O	1:A:29:TYR:CG	0.50	2.64	12	5
1:A:5:SER:O	1:A:9:LYS:N	0.50	2.45	14	1
1:A:27:ASP:CB	1:A:29:TYR:CZ	0.50	2.95	6	4
1:A:35:CYS:SG	1:A:36:LEU:N	0.49	2.86	4	1
1:A:38:ASN:HB3	1:A:59:ILE:CD1	0.49	2.37	11	5
1:A:58:PRO:O	1:A:59:ILE:HG23	0.49	2.06	2	1
1:A:9:LYS:CB	1:A:9:LYS:HZ2	0.49	2.19	14	1
1:A:29:TYR:CZ	1:A:38:ASN:OD1	0.49	2.66	1	2
1:A:27:ASP:CG	1:A:38:ASN:ND2	0.49	2.70	10	1
1:A:29:TYR:CE1	1:A:65:GLU:HB2	0.49	2.43	10	1
1:A:10:PRO:O	1:A:11:HIS:C	0.49	2.56	15	1
1:A:38:ASN:OD1	1:A:59:ILE:HD12	0.49	2.08	8	2
1:A:48:ASP:OD1	1:A:48:ASP:N	0.49	2.44	7	2
1:A:51:GLN:C	1:A:52:CYS:SG	0.48	2.96	1	3
1:A:60:GLY:HA3	1:A:64:PRO:HG2	0.48	1.85	14	6
1:A:6:CYS:SG	1:A:60:GLY:O	0.48	2.71	9	5
1:A:44:VAL:HG22	1:A:53:TYR:O	0.48	2.08	3	1
1:A:38:ASN:OD1	1:A:59:ILE:CD1	0.48	2.62	11	1
1:A:11:HIS:HA	1:A:58:PRO:CD	0.48	2.39	1	9
1:A:25:THR:O	1:A:65:GLU:CG	0.48	2.62	12	1
1:A:16:PHE:CZ	1:A:31:ASN:OD1	0.48	2.66	6	1
1:A:3:VAL:HG12	1:A:7:LEU:HD12	0.48	1.83	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:CYS:C	1:A:61:LEU:O	0.48	2.56	10	5
1:A:36:LEU:HB2	1:A:62:ALA:C	0.48	2.33	11	2
1:A:37:TRP:O	1:A:59:ILE:HD11	0.48	2.08	15	1
1:A:51:GLN:O	1:A:52:CYS:SG	0.48	2.72	6	4
1:A:27:ASP:HB2	1:A:29:TYR:OH	0.48	2.08	12	7
1:A:55:THR:C	1:A:56:TRP:CD1	0.48	2.92	12	3
1:A:22:ASP:OD2	1:A:25:THR:OG1	0.48	2.30	12	1
1:A:63:ILE:O	1:A:65:GLU:CD	0.48	2.56	13	1
1:A:18:ASN:N	1:A:50:THR:O	0.48	2.47	15	2
1:A:32:TYR:O	1:A:33:GLU:O	0.48	2.32	1	7
1:A:36:LEU:HG	1:A:62:ALA:O	0.48	2.08	6	3
1:A:16:PHE:CE2	1:A:31:ASN:O	0.48	2.66	9	1
1:A:29:TYR:CZ	1:A:65:GLU:HB2	0.48	2.43	10	1
1:A:16:PHE:HB3	1:A:30:ALA:CB	0.48	2.39	13	6
1:A:36:LEU:HD22	1:A:63:ILE:HA	0.48	1.85	15	1
1:A:20:TRP:CZ2	1:A:29:TYR:CD2	0.48	3.01	10	1
1:A:63:ILE:O	1:A:65:GLU:OE2	0.48	2.31	13	1
1:A:10:PRO:O	1:A:12:THR:N	0.48	2.46	15	1
1:A:58:PRO:O	1:A:59:ILE:CG2	0.47	2.61	2	1
1:A:29:TYR:HD1	1:A:36:LEU:HD11	0.47	1.67	6	3
1:A:37:TRP:HB3	1:A:56:TRP:O	0.47	2.09	15	15
1:A:44:VAL:O	1:A:52:CYS:SG	0.47	2.72	11	4
1:A:20:TRP:CZ2	1:A:63:ILE:HD11	0.47	2.44	14	2
1:A:38:ASN:OD1	1:A:57:VAL:O	0.47	2.32	12	3
1:A:48:ASP:O	1:A:49:GLU:CD	0.47	2.58	12	1
1:A:36:LEU:HD13	1:A:59:ILE:CD1	0.47	2.31	14	1
1:A:25:THR:HB	1:A:65:GLU:CB	0.47	2.39	14	5
1:A:52:CYS:HB3	1:A:56:TRP:CZ2	0.47	2.44	11	3
1:A:42:VAL:O	1:A:42:VAL:CG1	0.47	2.57	12	1
1:A:22:ASP:HB3	1:A:25:THR:OG1	0.47	2.10	2	9
1:A:13:GLU:O	1:A:14:ASN:CB	0.47	2.61	12	8
1:A:20:TRP:CH2	1:A:36:LEU:CD1	0.47	2.97	4	2
1:A:25:THR:O	1:A:65:GLU:CD	0.47	2.56	12	1
1:A:29:TYR:OH	1:A:65:GLU:HG3	0.47	2.09	12	1
1:A:14:ASN:HB2	1:A:37:TRP:CZ3	0.47	2.45	14	1
1:A:27:ASP:O	1:A:29:TYR:CE1	0.47	2.68	15	3
1:A:5:SER:O	1:A:6:CYS:C	0.47	2.57	13	6
1:A:40:THR:O	1:A:41:GLY:O	0.47	2.33	10	1
1:A:26:LEU:O	1:A:27:ASP:CG	0.47	2.57	13	1
1:A:34:GLY:O	1:A:61:LEU:O	0.47	2.33	8	1
1:A:25:THR:CB	1:A:65:GLU:CD	0.47	2.88	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ALA:O	1:A:63:ILE:HG12	0.47	2.09	13	11
1:A:25:THR:CB	1:A:65:GLU:HB3	0.47	2.40	2	4
1:A:29:TYR:CD2	1:A:36:LEU:HD23	0.47	2.44	15	1
1:A:31:ASN:O	1:A:31:ASN:ND2	0.47	2.48	15	1
1:A:64:PRO:O	1:A:65:GLU:HB3	0.47	2.09	15	1
1:A:28:ARG:CG	1:A:39:ALA:HB3	0.47	2.40	15	3
1:A:39:ALA:O	1:A:40:THR:O	0.47	2.33	7	1
1:A:15:SER:HB2	1:A:53:TYR:HA	0.46	1.87	2	2
1:A:19:VAL:CG1	1:A:20:TRP:N	0.46	2.78	11	3
1:A:38:ASN:HB3	1:A:57:VAL:HG23	0.46	1.87	1	1
1:A:18:ASN:O	1:A:19:VAL:C	0.46	2.57	6	8
1:A:7:LEU:O	1:A:8:ALA:C	0.46	2.57	6	1
1:A:20:TRP:CZ3	1:A:29:TYR:HB3	0.46	2.45	10	1
1:A:9:LYS:HE3	1:A:37:TRP:CZ2	0.46	2.45	2	3
1:A:36:LEU:HD13	1:A:36:LEU:C	0.46	2.36	6	2
1:A:45:CYS:SG	1:A:51:GLN:C	0.46	2.98	8	1
1:A:40:THR:OG1	1:A:41:GLY:N	0.46	2.46	1	4
1:A:48:ASP:O	1:A:49:GLU:OE1	0.46	2.33	4	1
1:A:31:ASN:O	1:A:31:ASN:OD1	0.46	2.33	7	3
1:A:45:CYS:CB	1:A:49:GLU:OE1	0.46	2.63	8	1
1:A:38:ASN:HB2	1:A:59:ILE:HD12	0.46	1.87	13	2
1:A:20:TRP:CH2	1:A:63:ILE:HA	0.46	2.46	4	3
1:A:60:GLY:HA3	1:A:64:PRO:CG	0.46	2.41	11	3
1:A:26:LEU:O	1:A:27:ASP:OD1	0.46	2.33	11	1
1:A:64:PRO:O	1:A:65:GLU:OE1	0.46	2.34	15	1
1:A:48:ASP:O	1:A:49:GLU:HB2	0.46	2.11	4	11
1:A:45:CYS:SG	1:A:51:GLN:O	0.46	2.73	8	1
1:A:12:THR:CG2	1:A:55:THR:HB	0.46	2.41	13	7
1:A:26:LEU:O	1:A:27:ASP:HB2	0.46	2.11	15	10
1:A:20:TRP:CZ3	1:A:36:LEU:CD1	0.46	2.98	4	1
1:A:18:ASN:O	1:A:19:VAL:O	0.46	2.33	6	2
1:A:36:LEU:CB	1:A:64:PRO:HD2	0.46	2.40	11	1
1:A:59:ILE:HG12	1:A:60:GLY:N	0.45	2.26	12	4
1:A:20:TRP:CD1	1:A:21:LYS:O	0.45	2.69	12	1
1:A:3:VAL:CG2	1:A:7:LEU:CD1	0.45	2.94	14	1
1:A:9:LYS:NZ	1:A:58:PRO:HB3	0.45	2.25	14	1
1:A:10:PRO:O	1:A:11:HIS:HB2	0.45	2.10	9	14
1:A:43:VAL:HG12	1:A:52:CYS:HB3	0.45	1.86	1	1
1:A:5:SER:HA	1:A:8:ALA:HB3	0.45	1.88	3	2
1:A:23:ASP:OD1	1:A:23:ASP:O	0.45	2.34	12	2
1:A:46:THR:HG23	1:A:51:GLN:OE1	0.45	2.11	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:CD1	1:A:59:ILE:CD1	0.45	2.94	2	3
1:A:63:ILE:O	1:A:63:ILE:CG1	0.45	2.64	11	1
1:A:25:THR:O	1:A:65:GLU:HG3	0.45	2.12	12	1
1:A:29:TYR:OH	1:A:65:GLU:HG2	0.45	2.10	12	1
1:A:41:GLY:O	1:A:43:VAL:HG23	0.45	2.11	14	2
1:A:27:ASP:HB3	1:A:38:ASN:OD1	0.45	2.10	3	4
1:A:36:LEU:CD1	1:A:37:TRP:O	0.45	2.64	1	3
1:A:12:THR:HG23	1:A:55:THR:CB	0.45	2.42	11	7
1:A:6:CYS:O	1:A:58:PRO:HB2	0.45	2.12	14	2
1:A:40:THR:HG23	1:A:41:GLY:H	0.45	1.71	14	2
1:A:3:VAL:HG22	1:A:7:LEU:HD12	0.45	1.86	14	1
1:A:3:VAL:O	1:A:7:LEU:HG	0.45	2.11	10	14
1:A:36:LEU:HG	1:A:63:ILE:N	0.45	2.26	12	3
1:A:7:LEU:HD21	1:A:60:GLY:N	0.45	2.27	6	1
1:A:44:VAL:O	1:A:52:CYS:HB3	0.45	2.11	8	2
1:A:45:CYS:CA	1:A:52:CYS:HB3	0.45	2.42	8	1
1:A:15:SER:HB3	1:A:53:TYR:HA	0.45	1.88	4	10
1:A:62:ALA:O	1:A:63:ILE:CG1	0.45	2.65	13	3
1:A:49:GLU:O	1:A:50:THR:C	0.45	2.58	5	3
1:A:6:CYS:SG	1:A:34:GLY:O	0.45	2.75	6	2
1:A:38:ASN:O	1:A:38:ASN:CG	0.45	2.60	6	3
1:A:29:TYR:CD1	1:A:38:ASN:CB	0.45	2.99	8	1
1:A:36:LEU:HD13	1:A:59:ILE:CG1	0.45	2.42	11	1
1:A:38:ASN:N	1:A:57:VAL:O	0.45	2.50	13	6
1:A:36:LEU:HD22	1:A:64:PRO:HD2	0.45	1.88	15	1
1:A:12:THR:HG22	1:A:13:GLU:N	0.45	2.27	3	7
1:A:42:VAL:O	1:A:43:VAL:CG2	0.45	2.65	8	1
1:A:9:LYS:CE	1:A:35:CYS:SG	0.44	3.05	2	4
1:A:9:LYS:HE2	1:A:35:CYS:SG	0.44	2.53	6	4
1:A:36:LEU:C	1:A:36:LEU:HD22	0.44	2.37	2	1
1:A:45:CYS:HA	1:A:51:GLN:O	0.44	2.12	8	2
1:A:15:SER:HA	1:A:56:TRP:NE1	0.44	2.27	15	14
1:A:8:ALA:C	1:A:9:LYS:O	0.44	2.60	2	11
1:A:20:TRP:CZ2	1:A:29:TYR:CB	0.44	3.01	2	1
1:A:25:THR:HB	1:A:65:GLU:HB3	0.44	1.90	9	7
1:A:48:ASP:C	1:A:49:GLU:HG3	0.44	2.37	2	3
1:A:11:HIS:O	1:A:12:THR:CG2	0.44	2.65	1	8
1:A:15:SER:HG	1:A:53:TYR:HA	0.44	1.72	2	2
1:A:36:LEU:HB3	1:A:60:GLY:C	0.44	2.38	3	1
1:A:44:VAL:O	1:A:52:CYS:HA	0.44	2.11	11	3
1:A:48:ASP:C	1:A:49:GLU:CG	0.44	2.91	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:PHE:CE2	1:A:31:ASN:ND2	0.43	2.85	15	1
1:A:12:THR:HG23	1:A:13:GLU:N	0.43	2.29	14	7
1:A:43:VAL:O	1:A:52:CYS:SG	0.43	2.76	13	2
1:A:36:LEU:CG	1:A:64:PRO:HD2	0.43	2.43	11	1
1:A:47:GLY:O	1:A:48:ASP:CB	0.43	2.66	6	3
1:A:45:CYS:N	1:A:52:CYS:SG	0.43	2.91	9	2
1:A:36:LEU:HD13	1:A:63:ILE:H	0.43	1.71	15	1
1:A:65:GLU:CD	1:A:65:GLU:C	0.43	2.87	10	1
1:A:36:LEU:HD22	1:A:36:LEU:C	0.43	2.38	11	1
1:A:7:LEU:O	1:A:58:PRO:HG2	0.43	2.12	6	1
1:A:6:CYS:O	1:A:9:LYS:HE3	0.43	2.13	14	1
1:A:45:CYS:HB3	1:A:49:GLU:CB	0.43	2.43	6	1
1:A:59:ILE:HG13	1:A:65:GLU:O	0.43	2.14	14	1
1:A:58:PRO:C	1:A:59:ILE:HG23	0.43	2.39	2	1
1:A:3:VAL:O	1:A:7:LEU:CG	0.43	2.66	8	4
1:A:16:PHE:HD2	1:A:19:VAL:HG22	0.43	1.73	6	1
1:A:27:ASP:CB	1:A:29:TYR:OH	0.43	2.67	12	1
1:A:28:ARG:O	1:A:38:ASN:HA	0.43	2.14	10	4
1:A:47:GLY:O	1:A:48:ASP:HB2	0.42	2.14	9	6
1:A:28:ARG:C	1:A:29:TYR:CD2	0.42	2.97	1	1
1:A:15:SER:OG	1:A:16:PHE:N	0.42	2.51	2	2
1:A:50:THR:CG2	1:A:51:GLN:N	0.42	2.81	3	1
1:A:5:SER:C	1:A:7:LEU:N	0.42	2.77	6	2
1:A:28:ARG:NH1	1:A:28:ARG:HG3	0.42	2.28	8	1
1:A:43:VAL:CG1	1:A:54:GLY:HA3	0.42	2.44	3	1
1:A:52:CYS:HB3	1:A:56:TRP:CH2	0.42	2.49	15	1
1:A:28:ARG:HB3	1:A:39:ALA:O	0.42	2.15	6	2
1:A:29:TYR:OH	1:A:65:GLU:HB2	0.42	2.14	10	1
1:A:28:ARG:C	1:A:29:TYR:CG	0.42	2.97	12	1
1:A:3:VAL:HA	1:A:61:LEU:HD21	0.42	1.91	15	1
1:A:25:THR:HG21	1:A:63:ILE:HG23	0.42	1.90	15	1
1:A:16:PHE:CG	1:A:17:THR:N	0.42	2.87	2	1
1:A:36:LEU:HD22	1:A:63:ILE:CA	0.42	2.44	9	2
1:A:15:SER:OG	1:A:53:TYR:HA	0.42	2.15	2	2
1:A:17:THR:O	1:A:18:ASN:HB3	0.42	2.14	13	1
1:A:19:VAL:CG1	1:A:29:TYR:O	0.42	2.68	3	1
1:A:14:ASN:O	1:A:15:SER:HB3	0.42	2.15	11	2
1:A:17:THR:O	1:A:18:ASN:HB2	0.42	2.14	11	1
1:A:43:VAL:CG1	1:A:56:TRP:CZ2	0.42	3.03	13	2
1:A:36:LEU:CD2	1:A:64:PRO:CD	0.42	2.98	15	1
1:A:45:CYS:HB3	1:A:49:GLU:CG	0.42	2.44	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ALA:O	1:A:9:LYS:C	0.42	2.62	6	1
1:A:18:ASN:O	1:A:18:ASN:CG	0.42	2.62	15	1
1:A:64:PRO:C	1:A:65:GLU:HG2	0.42	2.39	15	1
1:A:20:TRP:CD1	1:A:20:TRP:C	0.41	2.95	2	2
1:A:39:ALA:CB	1:A:56:TRP:CZ3	0.41	2.99	2	1
1:A:6:CYS:O	1:A:9:LYS:HD2	0.41	2.14	4	1
1:A:20:TRP:CE3	1:A:29:TYR:HB2	0.41	2.50	10	1
1:A:20:TRP:CD1	1:A:21:LYS:C	0.41	2.98	11	1
1:A:37:TRP:C	1:A:59:ILE:CD1	0.41	2.93	15	1
1:A:25:THR:HA	1:A:65:GLU:HB3	0.41	1.91	11	2
1:A:10:PRO:O	1:A:11:HIS:CB	0.41	2.68	13	2
1:A:19:VAL:CG2	1:A:56:TRP:CH2	0.41	2.99	13	1
1:A:38:ASN:HB3	1:A:57:VAL:O	0.41	2.15	13	1
1:A:38:ASN:OD1	1:A:57:VAL:HB	0.41	2.15	8	1
1:A:45:CYS:HB3	1:A:49:GLU:CA	0.41	2.44	11	1
1:A:63:ILE:H	1:A:64:PRO:CD	0.41	2.27	12	1
1:A:25:THR:HB	1:A:65:GLU:HA	0.41	1.93	14	1
1:A:34:GLY:O	1:A:61:LEU:HA	0.41	2.15	9	1
1:A:3:VAL:CG2	1:A:7:LEU:HD11	0.41	2.43	10	1
1:A:32:TYR:HB2	1:A:35:CYS:O	0.41	2.15	9	1
1:A:52:CYS:HB2	1:A:56:TRP:CZ2	0.41	2.51	14	1
1:A:11:HIS:HA	1:A:58:PRO:HD3	0.41	1.92	15	2
1:A:43:VAL:HB	1:A:52:CYS:SG	0.41	2.56	9	1
1:A:15:SER:OG	1:A:52:CYS:O	0.41	2.34	10	1
1:A:29:TYR:OH	1:A:65:GLU:CB	0.41	2.68	10	1
1:A:6:CYS:C	1:A:9:LYS:HG3	0.41	2.41	11	1
1:A:36:LEU:HB2	1:A:62:ALA:HA	0.41	1.93	12	1
1:A:61:LEU:N	1:A:61:LEU:HD23	0.41	2.29	13	1
1:A:25:THR:CA	1:A:65:GLU:HB3	0.40	2.46	7	1
1:A:29:TYR:CG	1:A:36:LEU:HD21	0.40	2.51	15	1
1:A:30:ALA:HB2	1:A:56:TRP:CE3	0.40	2.50	15	1
1:A:23:ASP:O	1:A:26:LEU:HD22	0.40	2.16	9	1
1:A:43:VAL:O	1:A:44:VAL:C	0.40	2.63	13	1
1:A:9:LYS:HD2	1:A:35:CYS:SG	0.40	2.56	4	1
1:A:36:LEU:CD1	1:A:59:ILE:HG13	0.40	2.46	11	1
1:A:31:ASN:HA	1:A:36:LEU:CD2	0.40	2.46	5	1
1:A:7:LEU:HD21	1:A:59:ILE:C	0.40	2.42	6	1
1:A:32:TYR:O	1:A:32:TYR:CD2	0.40	2.74	8	1
1:A:32:TYR:CB	1:A:35:CYS:O	0.40	2.70	9	1
1:A:22:ASP:CG	1:A:29:TYR:CD1	0.40	2.99	12	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	63/70 (90%)	42±2 (67±3%)	11±2 (18±3%)	10±2 (15±3%)	0 4
All	All	945/1050 (90%)	633 (67%)	168 (18%)	144 (15%)	0 4

All 18 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	9	LYS	15
1	A	13	GLU	15
1	A	14	ASN	15
1	A	63	ILE	13
1	A	27	ASP	13
1	A	33	GLU	11
1	A	62	ALA	11
1	A	19	VAL	11
1	A	12	THR	8
1	A	65	GLU	7
1	A	59	ILE	6
1	A	41	GLY	5
1	A	42	VAL	4
1	A	44	VAL	4
1	A	40	THR	2
1	A	26	LEU	2
1	A	11	HIS	1
1	A	64	PRO	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	54/58 (93%)	37±2 (68±4%)	17±2 (32±4%)	1	13
All	All	810/870 (93%)	548 (68%)	262 (32%)	1	13

All 37 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	12	THR	15
1	A	17	THR	15
1	A	59	ILE	15
1	A	20	TRP	14
1	A	27	ASP	14
1	A	63	ILE	14
1	A	38	ASN	13
1	A	14	ASN	11
1	A	22	ASP	11
1	A	11	HIS	11
1	A	50	THR	11
1	A	21	LYS	10
1	A	26	LEU	9
1	A	52	CYS	8
1	A	24	LYS	7
1	A	35	CYS	7
1	A	40	THR	7
1	A	43	VAL	7
1	A	3	VAL	6
1	A	48	ASP	5
1	A	49	GLU	5
1	A	51	GLN	5
1	A	6	CYS	4
1	A	28	ARG	4
1	A	53	TYR	4
1	A	65	GLU	4
1	A	36	LEU	4
1	A	4	GLU	4
1	A	33	GLU	4
1	A	57	VAL	3
1	A	5	SER	3
1	A	9	LYS	2
1	A	23	ASP	2
1	A	18	ASN	1
1	A	45	CYS	1
1	A	46	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	31	ASN	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 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