



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 1RML / pdb_00001rml
Title : NMR STUDY OF ACID FIBROBLAST GROWTH FACTOR BOUND TO
1,3,6-NAPHTHALENE TRISULPHONATE, 26 STRUCTURES
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Deposited on : 1998-05-21

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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

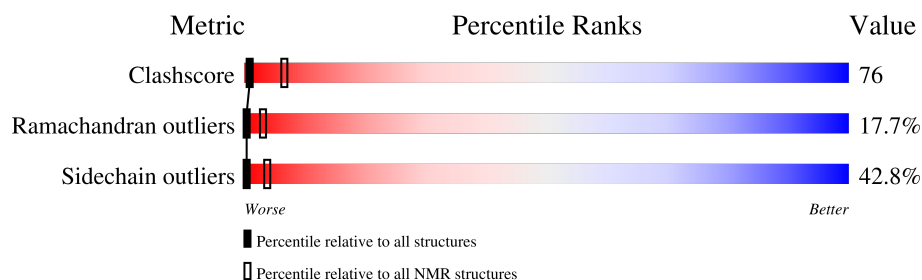
1 Overall quality at a glance

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	155	

2 Ensemble composition and analysis

This entry contains 26 models. Model 3 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:26-A:31, A:35-A:139, A:144-A:151 (119)	0.65	3

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 7, 8, 10, 12, 13, 14, 15, 17, 18, 19, 21, 25, 26
2	2, 4, 5, 9, 16, 20, 23, 24
3	11, 22

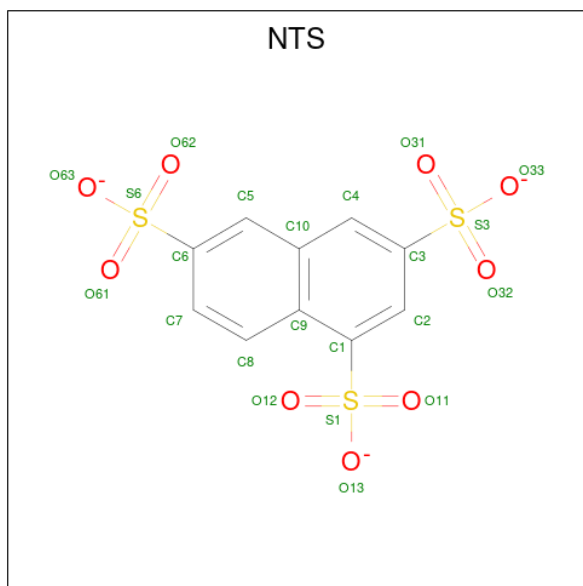
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2091 atoms, of which 1027 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ACIDIC FIBROBLAST GROWTH FACTOR.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			2064	656	1022	182	200	4	

- Molecule 2 is NAPHTHALENE TRISULFONATE (CCD ID: NTS) (formula: $C_{10}H_5O_9S_3$).



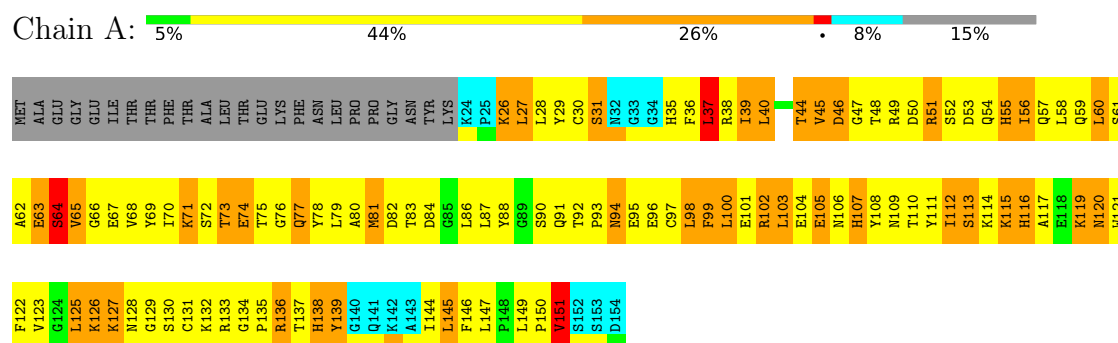
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	O	S
			27	10	5	9	3

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: ACIDIC FIBROBLAST GROWTH FACTOR

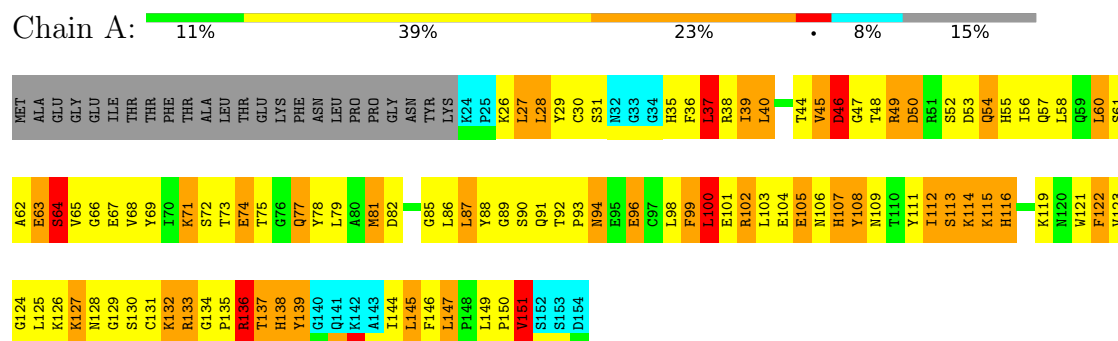


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

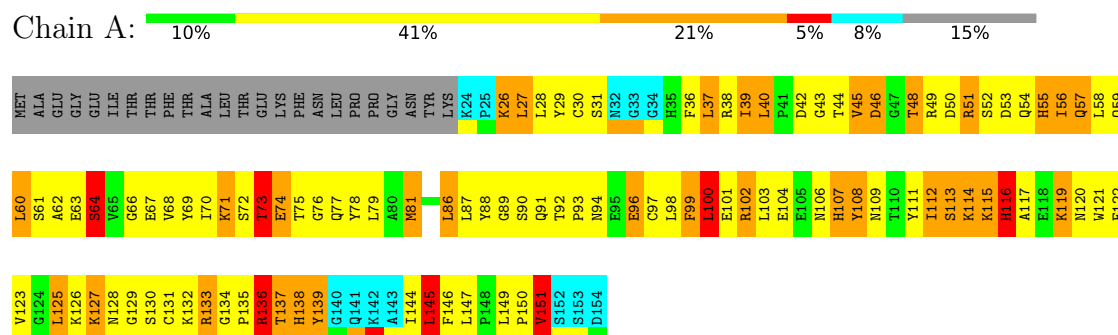
4.2.1 Score per residue for model 1

• Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



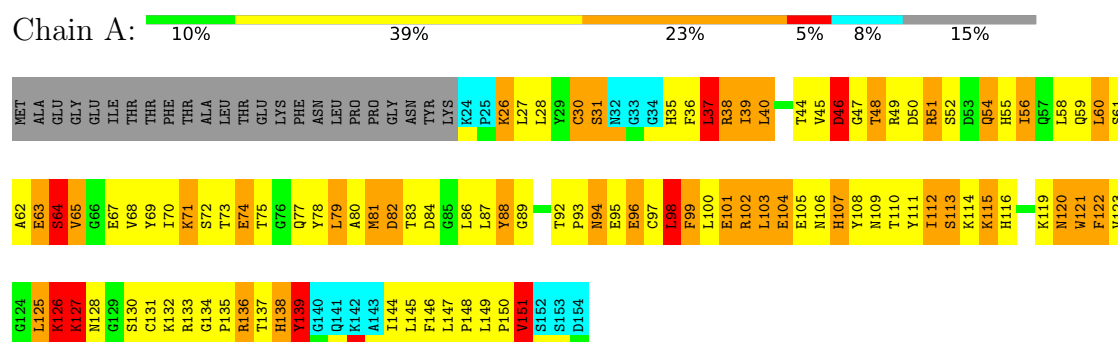
4.2.2 Score per residue for model 2

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



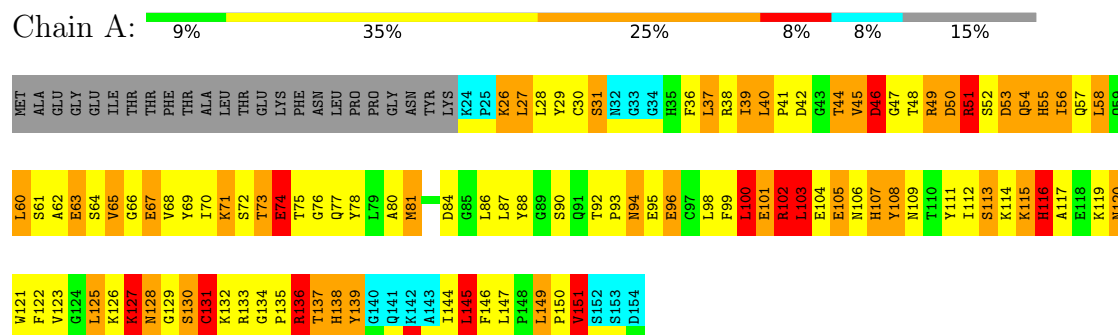
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



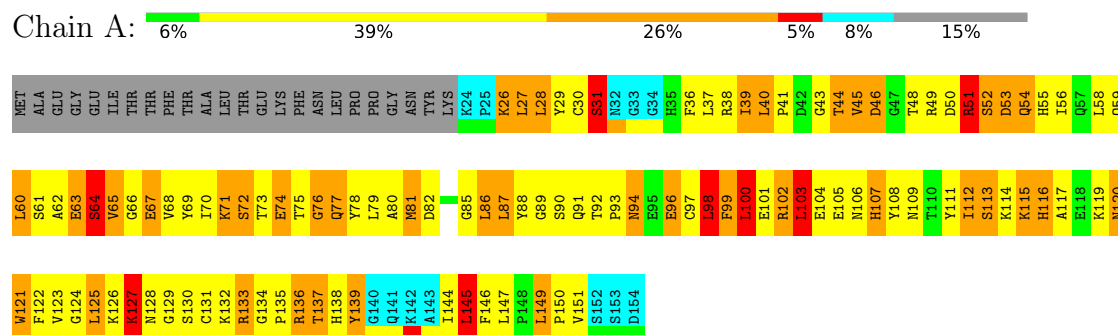
4.2.4 Score per residue for model 4

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



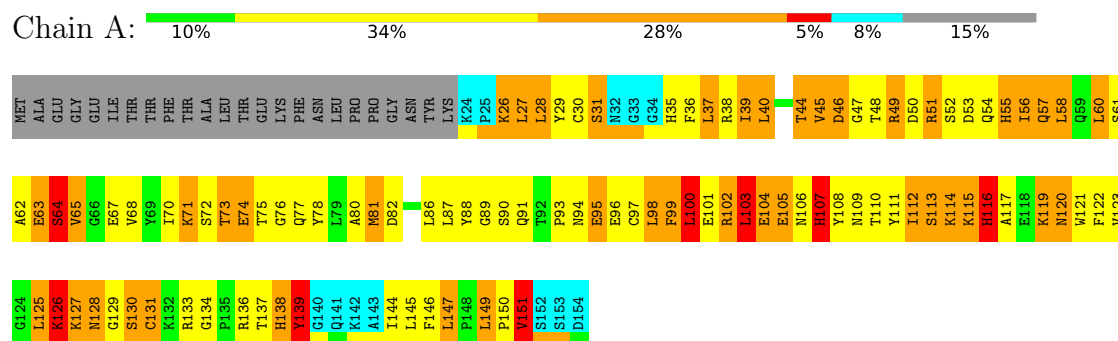
4.2.5 Score per residue for model 5

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



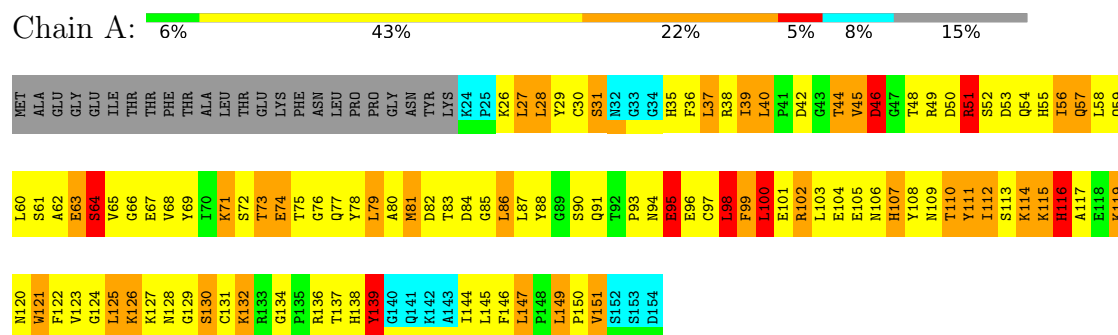
4.2.6 Score per residue for model 6

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.7 Score per residue for model 7

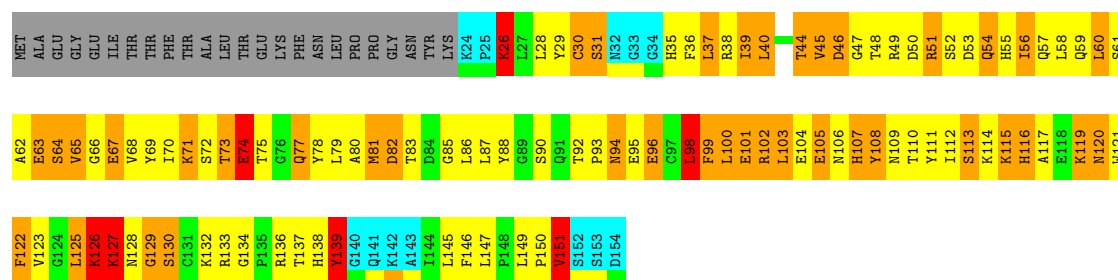
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.8 Score per residue for model 8

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

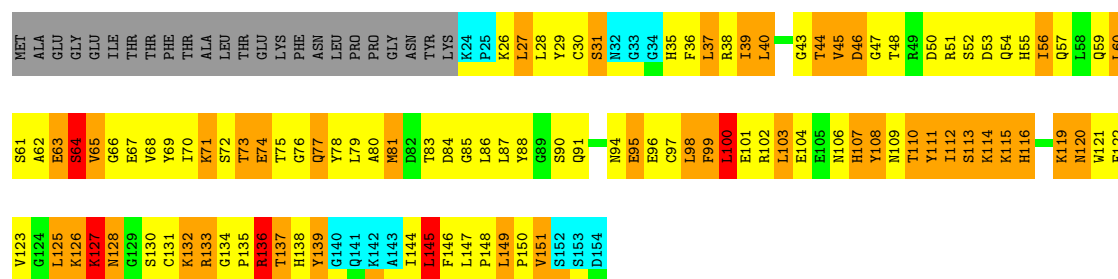




4.2.9 Score per residue for model 9

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

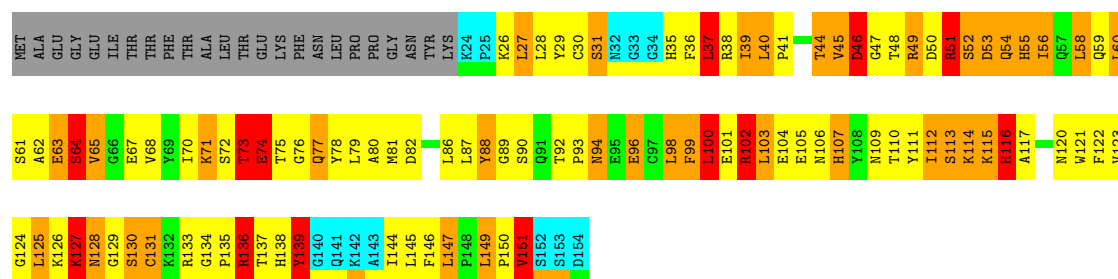
Chain A: 8% 39% 26% 8% 15%



4.2.10 Score per residue for model 10

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

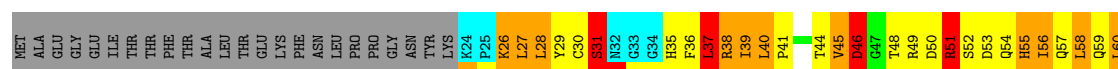
Chain A: 10% 35% 23% 8% 8% 15%

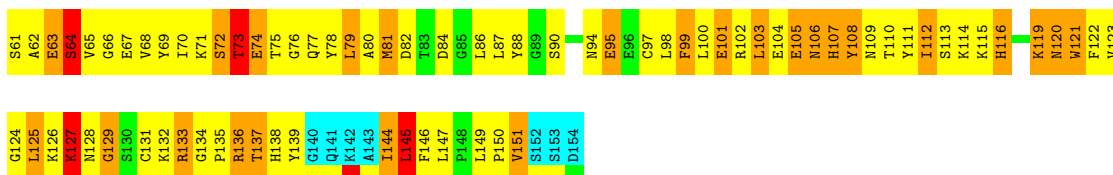


4.2.11 Score per residue for model 11

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

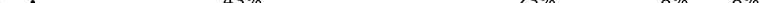
Chain A: 9% 39% 23% 5% 8% 15%

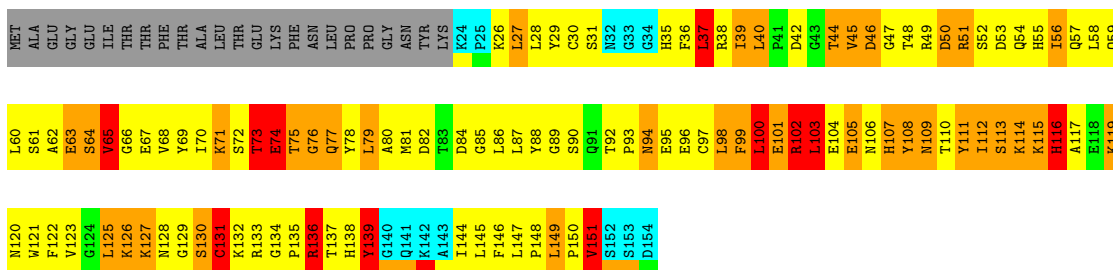




4.2.12 Score per residue for model 12

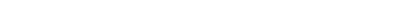
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

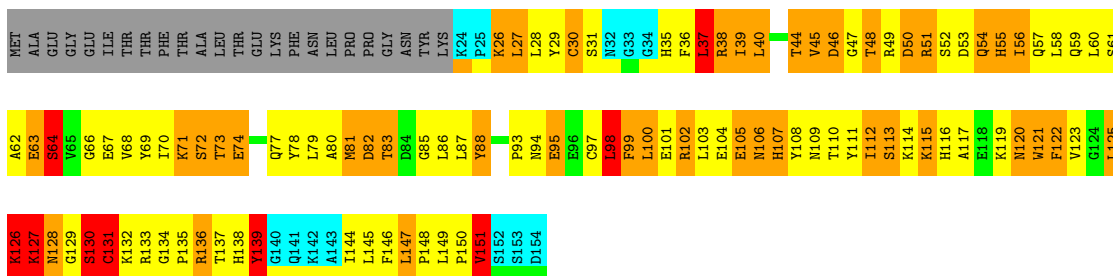
Chain A: 



4.2.13 Score per residue for model 13

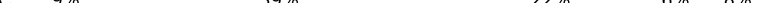
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

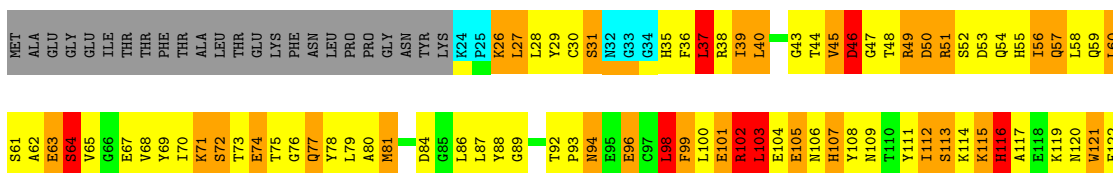
Chain A: 



4.2.14 Score per residue for model 14

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

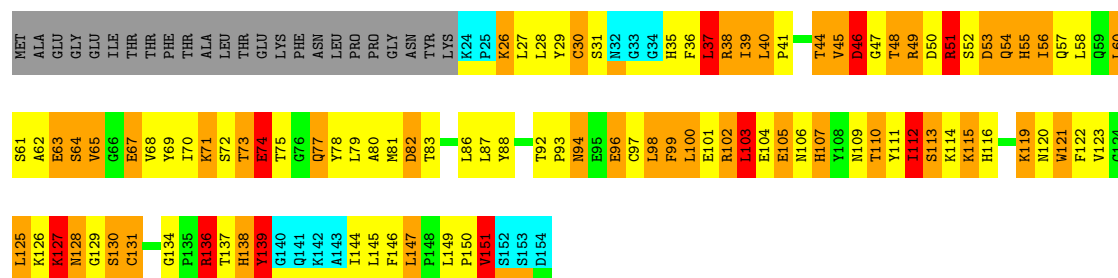
Chain A:  9% 39% 22% 6% 8% 15%





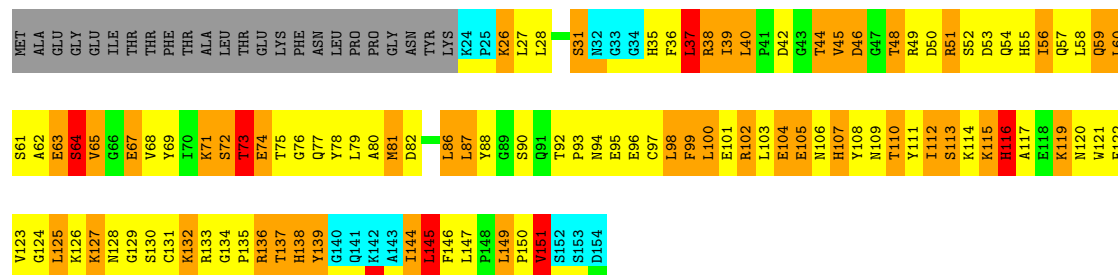
4.2.15 Score per residue for model 15

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



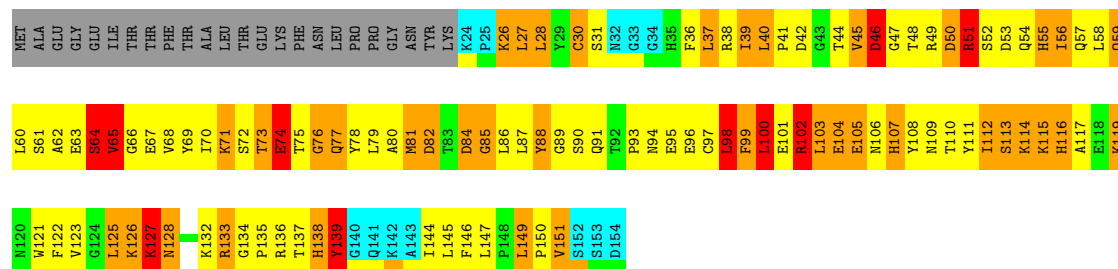
4.2.16 Score per residue for model 16

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



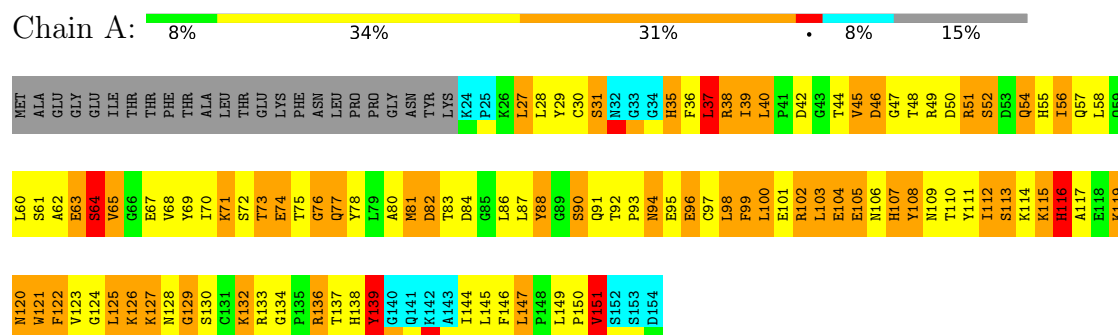
4.2.17 Score per residue for model 17

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



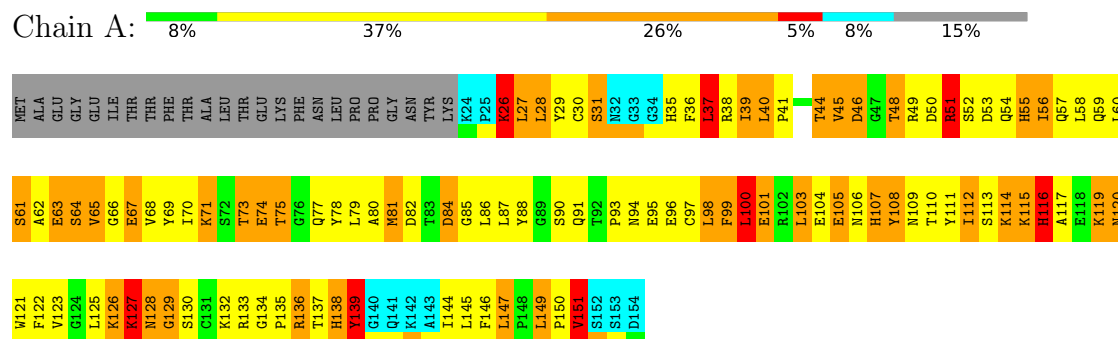
4.2.18 Score per residue for model 18

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



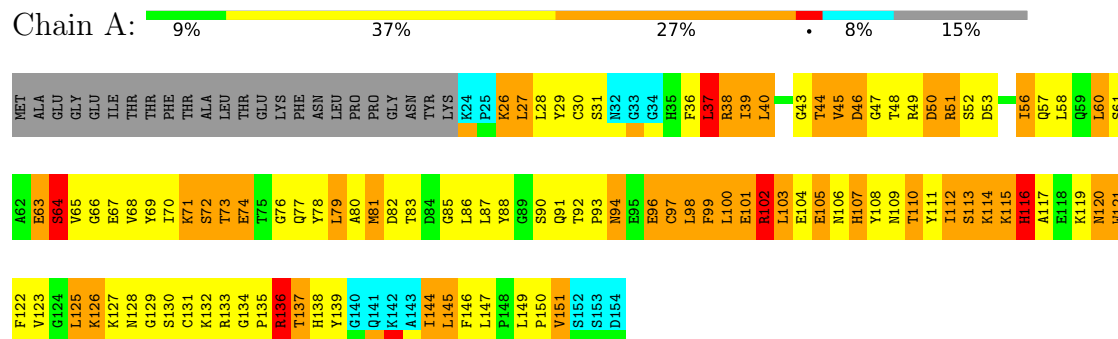
4.2.19 Score per residue for model 19

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



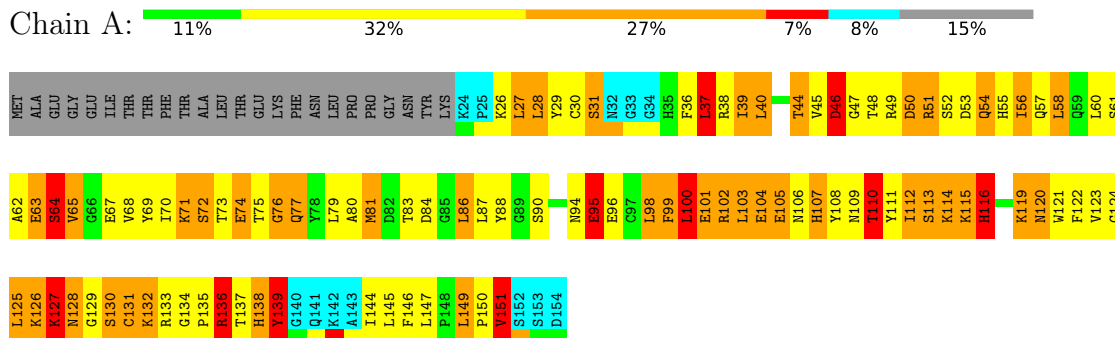
4.2.20 Score per residue for model 20

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



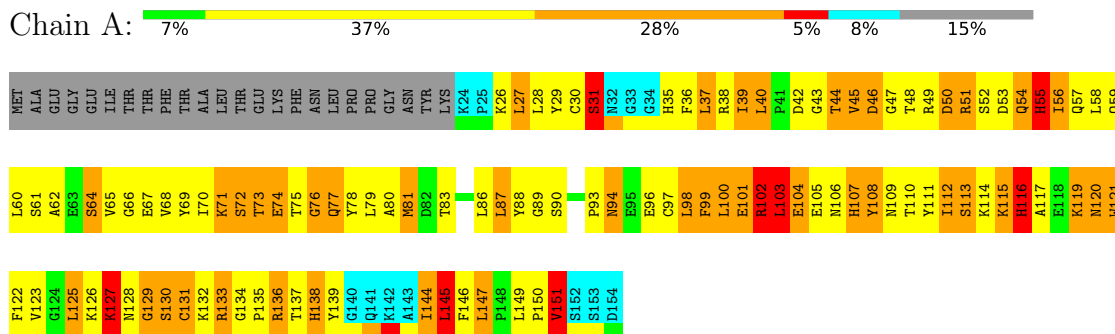
4.2.21 Score per residue for model 21

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



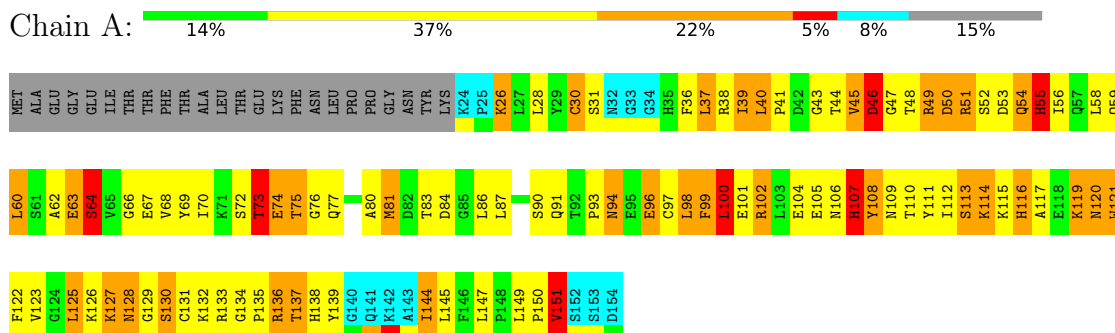
4.2.22 Score per residue for model 22

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.23 Score per residue for model 23

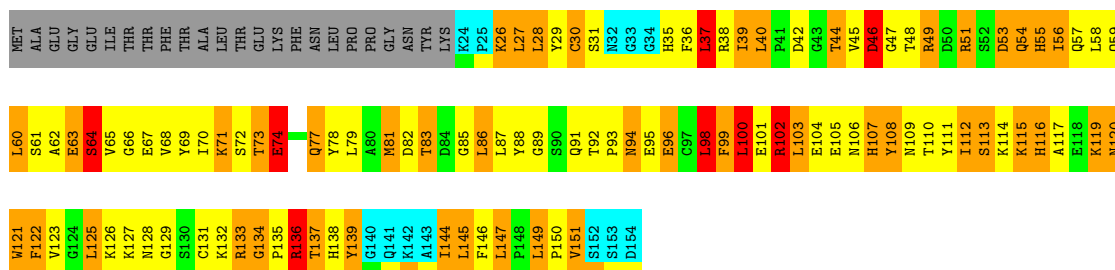
- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR



4.2.24 Score per residue for model 24

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

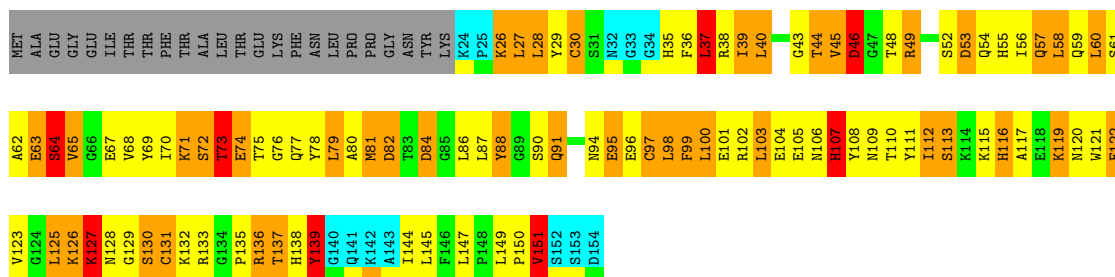




4.2.25 Score per residue for model 25

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

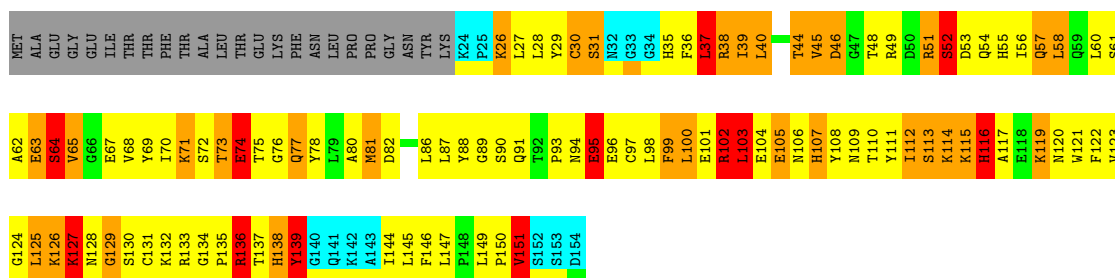
Chain A: 12% 34% 26% 5% 8% 15%



4.2.26 Score per residue for model 26

- Molecule 1: ACIDIC FIBROBLAST GROWTH FACTOR

Chain A: 9% 40% 20% 8% 8% 15%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *VARIABLE TARGET FUNCTION*.

Of the 26 calculated structures, 26 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA	refinement	
DIANA	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
NTS

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	963	947	947	147±14
2	A	22	5	5	3±2
All	All	25610	24752	24752	3826

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 76.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:ILE:HD11	1:A:122:PHE:CE1	1.07	1.84	12	14
1:A:108:TYR:CE2	1:A:145:LEU:HD23	0.96	1.95	25	3
1:A:108:TYR:CD2	1:A:145:LEU:HD23	0.91	2.00	3	7
1:A:37:LEU:HD23	1:A:125:LEU:HD21	0.90	1.43	8	2
1:A:70:ILE:HD12	1:A:99:PHE:CD2	0.89	2.01	24	13
1:A:112:ILE:HD11	1:A:122:PHE:CE2	0.89	2.02	14	5
1:A:68:VAL:O	1:A:98:LEU:HD23	0.89	1.66	20	23
1:A:104:GLU:OE2	1:A:145:LEU:HD21	0.89	1.67	25	3
1:A:69:TYR:CZ	1:A:98:LEU:HD21	0.88	2.02	2	3
1:A:87:LEU:HD21	1:A:123:VAL:HG23	0.88	1.41	14	15
1:A:81:MET:HE1	1:A:122:PHE:O	0.88	1.69	7	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLU:CD	1:A:145:LEU:HD21	0.87	1.92	19	5
1:A:60:LEU:HD23	1:A:111:TYR:OH	0.86	1.71	1	5
1:A:104:GLU:OE1	1:A:145:LEU:HD21	0.86	1.71	7	2
1:A:37:LEU:HD12	1:A:146:PHE:CZ	0.86	2.06	12	17
1:A:47:GLY:N	1:A:125:LEU:HD22	0.86	1.86	12	11
1:A:29:TYR:CD1	1:A:36:PHE:CZ	0.85	2.63	7	12
1:A:28:LEU:HD21	1:A:146:PHE:HB3	0.84	1.49	14	7
1:A:79:LEU:HD11	1:A:87:LEU:HD23	0.84	1.46	1	2
1:A:87:LEU:HD21	1:A:123:VAL:CG2	0.83	2.04	23	13
1:A:108:TYR:CE2	1:A:145:LEU:HD13	0.83	2.07	23	2
1:A:112:ILE:HD11	1:A:122:PHE:CZ	0.83	2.08	23	9
1:A:144:ILE:HG13	1:A:145:LEU:HD12	0.82	1.50	18	4
1:A:81:MET:HE2	1:A:85:GLY:O	0.82	1.74	9	3
1:A:108:TYR:CD2	1:A:145:LEU:HD13	0.82	2.09	20	2
1:A:122:PHE:CE2	1:A:144:ILE:HD12	0.81	2.10	22	13
1:A:150:PRO:O	1:A:151:VAL:HG13	0.81	1.76	6	25
1:A:56:ILE:O	1:A:56:ILE:HD12	0.81	1.76	25	5
1:A:68:VAL:HG21	1:A:111:TYR:CE2	0.81	2.11	26	5
1:A:83:THR:HG22	1:A:115:LYS:HE2	0.79	1.50	15	1
1:A:27:LEU:HD12	1:A:27:LEU:C	0.79	2.01	17	19
1:A:67:GLU:OE2	1:A:98:LEU:HD13	0.79	1.76	13	9
1:A:134:GLY:O	1:A:137:THR:HG22	0.79	1.78	24	3
1:A:39:ILE:HD11	1:A:79:LEU:HD13	0.79	1.54	24	6
1:A:67:GLU:HB2	1:A:98:LEU:HD22	0.79	1.55	15	3
1:A:63:GLU:HG2	1:A:98:LEU:HD21	0.78	1.55	3	15
1:A:39:ILE:HG21	1:A:72:SER:CB	0.78	2.08	2	8
1:A:56:ILE:C	1:A:56:ILE:HD12	0.78	2.03	7	1
1:A:37:LEU:HG	1:A:125:LEU:HD11	0.78	1.54	8	18
1:A:102:ARG:NH2	1:A:112:ILE:HD12	0.78	1.93	17	6
1:A:149:LEU:O	1:A:149:LEU:HD12	0.78	1.77	3	15
1:A:112:ILE:HD11	1:A:122:PHE:CD1	0.78	2.14	12	4
1:A:27:LEU:HD12	1:A:28:LEU:O	0.78	1.77	6	7
1:A:47:GLY:HA3	1:A:125:LEU:HD13	0.77	1.55	18	6
1:A:110:THR:CG2	1:A:145:LEU:HD23	0.77	2.07	6	5
1:A:116:HIS:CE1	1:A:121:TRP:CZ3	0.77	2.72	3	5
1:A:47:GLY:CA	1:A:125:LEU:HD22	0.77	2.10	8	9
1:A:29:TYR:CD1	1:A:36:PHE:CE1	0.77	2.72	18	5
1:A:68:VAL:O	1:A:98:LEU:HD13	0.77	1.80	12	2
1:A:56:ILE:O	1:A:58:LEU:HD12	0.77	1.79	13	11
1:A:81:MET:HG3	1:A:87:LEU:HD12	0.76	1.55	6	6
1:A:59:GLN:O	1:A:70:ILE:HG23	0.76	1.80	10	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:N	1:A:125:LEU:HD12	0.76	1.96	5	2
1:A:56:ILE:HD12	1:A:56:ILE:C	0.75	2.05	18	5
1:A:102:ARG:CZ	1:A:112:ILE:HD12	0.75	2.10	22	2
1:A:46:ASP:C	1:A:125:LEU:HD22	0.75	2.07	21	13
1:A:31:SER:HB3	1:A:145:LEU:HD23	0.75	1.59	12	1
1:A:27:LEU:HD12	1:A:27:LEU:O	0.74	1.81	16	9
1:A:139:TYR:O	1:A:139:TYR:CD2	0.74	2.41	9	1
1:A:37:LEU:HB3	1:A:58:LEU:HD13	0.74	1.57	23	3
1:A:39:ILE:CG1	1:A:45:VAL:HG13	0.74	2.12	23	3
1:A:40:LEU:HD12	1:A:55:HIS:CE1	0.74	2.17	15	1
1:A:67:GLU:HG2	1:A:98:LEU:HD22	0.73	1.58	17	18
1:A:139:TYR:CB	1:A:144:ILE:HD11	0.73	2.12	24	10
1:A:139:TYR:HB2	1:A:144:ILE:HD11	0.73	1.59	24	10
1:A:104:GLU:CD	1:A:145:LEU:HD22	0.73	2.09	11	2
1:A:83:THR:HG22	1:A:115:LYS:CE	0.73	2.12	15	1
1:A:28:LEU:HD23	1:A:29:TYR:N	0.73	1.98	14	4
1:A:39:ILE:HD12	1:A:45:VAL:HG13	0.73	1.58	25	5
1:A:68:VAL:C	1:A:98:LEU:HD23	0.73	2.08	3	22
1:A:27:LEU:HG	1:A:149:LEU:HD11	0.73	1.59	14	4
1:A:29:TYR:CE2	1:A:30:CYS:O	0.73	2.42	14	11
1:A:60:LEU:HD22	1:A:111:TYR:OH	0.72	1.83	16	6
1:A:133:ARG:O	1:A:134:GLY:C	0.72	2.33	24	15
1:A:37:LEU:CD2	1:A:125:LEU:HD21	0.72	2.13	8	6
1:A:39:ILE:CD1	1:A:45:VAL:HG13	0.72	2.14	25	3
1:A:68:VAL:HG11	1:A:101:GLU:OE1	0.72	1.85	15	4
1:A:121:TRP:HA	1:A:137:THR:HG23	0.72	1.61	24	3
1:A:37:LEU:HD11	1:A:146:PHE:CZ	0.71	2.19	16	3
1:A:60:LEU:HD22	1:A:111:TYR:CZ	0.70	2.21	14	2
1:A:39:ILE:HG12	1:A:45:VAL:HG13	0.70	1.64	23	1
1:A:108:TYR:CD2	1:A:145:LEU:CD1	0.70	2.75	12	2
1:A:37:LEU:CD1	1:A:146:PHE:CZ	0.70	2.75	8	14
1:A:40:LEU:HD12	1:A:44:THR:HB	0.70	1.62	11	5
1:A:75:THR:HG23	1:A:77:GLN:OE1	0.70	1.85	18	4
1:A:116:HIS:CG	1:A:121:TRP:CE3	0.70	2.80	3	4
1:A:81:MET:HE3	1:A:85:GLY:O	0.69	1.87	5	4
1:A:68:VAL:HG22	1:A:99:PHE:O	0.69	1.86	14	14
1:A:81:MET:HE1	1:A:137:THR:HG21	0.69	1.63	18	4
1:A:145:LEU:HD11	2:A:178:NTS:O61	0.69	1.87	18	2
1:A:59:GLN:OE1	1:A:60:LEU:HD12	0.69	1.87	11	1
1:A:145:LEU:HD23	1:A:145:LEU:N	0.69	2.03	5	6
1:A:116:HIS:ND1	1:A:121:TRP:CZ3	0.69	2.61	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:PHE:CZ	1:A:51:ARG:CZ	0.69	2.76	17	2
1:A:47:GLY:HA3	1:A:125:LEU:HD22	0.68	1.65	9	7
1:A:126:LYS:O	1:A:128:ASN:N	0.68	2.27	21	26
1:A:40:LEU:HD13	1:A:40:LEU:N	0.68	2.03	15	1
1:A:122:PHE:CZ	1:A:139:TYR:CD1	0.68	2.82	18	2
1:A:108:TYR:CD2	1:A:145:LEU:HD11	0.68	2.24	12	2
1:A:102:ARG:O	1:A:103:LEU:C	0.68	2.37	12	12
1:A:125:LEU:O	1:A:126:LYS:C	0.67	2.37	3	26
1:A:38:ARG:NH2	1:A:48:THR:HG21	0.67	2.04	4	8
1:A:62:ALA:CB	1:A:68:VAL:HG12	0.67	2.20	19	12
1:A:47:GLY:CA	1:A:125:LEU:HD13	0.67	2.20	23	3
1:A:139:TYR:CD2	2:A:178:NTS:O62	0.67	2.47	14	5
1:A:41:PRO:CD	1:A:55:HIS:CD2	0.67	2.78	10	1
1:A:69:TYR:CZ	1:A:98:LEU:CD2	0.66	2.77	12	3
1:A:115:LYS:CE	1:A:116:HIS:CD2	0.66	2.77	2	5
1:A:111:TYR:N	1:A:111:TYR:CD1	0.66	2.63	12	3
1:A:112:ILE:HD12	1:A:122:PHE:CE1	0.66	2.25	9	1
1:A:109:ASN:O	1:A:111:TYR:CE1	0.66	2.48	7	20
1:A:73:THR:HG23	1:A:73:THR:O	0.66	1.91	22	14
1:A:31:SER:CB	1:A:145:LEU:HD23	0.66	2.19	12	1
1:A:55:HIS:CE1	1:A:74:GLU:CD	0.66	2.74	14	5
1:A:60:LEU:N	1:A:60:LEU:HD12	0.66	2.06	2	2
1:A:112:ILE:CD1	1:A:122:PHE:CE1	0.66	2.73	12	4
1:A:147:LEU:O	1:A:149:LEU:HD23	0.65	1.91	10	5
1:A:139:TYR:CB	1:A:144:ILE:CD1	0.65	2.73	22	10
1:A:60:LEU:HD13	1:A:111:TYR:OH	0.65	1.91	24	6
1:A:139:TYR:CD1	1:A:144:ILE:CD1	0.65	2.79	14	5
1:A:60:LEU:HD12	1:A:60:LEU:H	0.65	1.50	2	3
1:A:67:GLU:HG2	1:A:98:LEU:HD12	0.65	1.66	2	2
1:A:116:HIS:ND1	1:A:121:TRP:CE3	0.65	2.64	24	5
1:A:144:ILE:CG1	1:A:145:LEU:HD12	0.65	2.21	14	3
1:A:109:ASN:O	1:A:111:TYR:CD1	0.65	2.50	6	20
1:A:37:LEU:HG	1:A:125:LEU:HD21	0.65	1.68	11	4
1:A:60:LEU:HD23	1:A:70:ILE:HG12	0.65	1.67	20	4
1:A:137:THR:C	1:A:138:HIS:CG	0.65	2.75	17	3
1:A:39:ILE:CD1	1:A:79:LEU:HD13	0.65	2.22	10	4
1:A:67:GLU:HB2	1:A:98:LEU:HD12	0.65	1.66	4	1
1:A:139:TYR:CD2	2:A:178:NTS:O61	0.65	2.49	15	2
1:A:35:HIS:CD2	1:A:49:ARG:N	0.65	2.64	11	4
1:A:39:ILE:HD12	1:A:45:VAL:CG1	0.65	2.21	25	2
1:A:28:LEU:HD23	1:A:29:TYR:H	0.65	1.52	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:LEU:HD11	1:A:107:HIS:N	0.65	2.07	10	1
1:A:108:TYR:CD2	1:A:145:LEU:HD22	0.65	2.27	19	2
1:A:139:TYR:CD2	2:A:178:NTS:O63	0.64	2.50	26	4
1:A:109:ASN:O	1:A:111:TYR:CD2	0.64	2.51	14	2
1:A:109:ASN:O	1:A:111:TYR:CE2	0.64	2.50	14	1
1:A:26:LYS:HZ2	1:A:58:LEU:C	0.64	2.00	8	1
1:A:27:LEU:HD11	1:A:149:LEU:HD11	0.64	1.69	1	1
1:A:86:LEU:HD12	1:A:133:ARG:HD3	0.63	1.71	1	1
1:A:81:MET:HE3	1:A:87:LEU:CD1	0.63	2.24	9	2
1:A:68:VAL:HG21	1:A:111:TYR:HE2	0.63	1.52	16	4
1:A:29:TYR:CZ	1:A:30:CYS:O	0.63	2.51	6	11
1:A:36:PHE:CD2	1:A:51:ARG:CG	0.63	2.82	18	3
1:A:106:ASN:C	1:A:107:HIS:CG	0.63	2.76	6	3
1:A:71:LYS:HZ2	1:A:72:SER:N	0.62	1.92	2	9
1:A:106:ASN:O	1:A:107:HIS:CD2	0.62	2.52	18	21
1:A:40:LEU:HD12	1:A:44:THR:O	0.62	1.94	26	6
1:A:139:TYR:HB3	1:A:144:ILE:CD1	0.62	2.24	2	10
1:A:82:ASP:O	1:A:116:HIS:CE1	0.62	2.52	1	2
1:A:39:ILE:C	1:A:40:LEU:HD13	0.62	2.19	15	9
1:A:50:ASP:O	1:A:51:ARG:C	0.62	2.43	19	17
1:A:103:LEU:HD11	1:A:106:ASN:HA	0.62	1.70	24	1
1:A:121:TRP:CD1	1:A:134:GLY:O	0.62	2.52	2	20
1:A:56:ILE:HD12	1:A:56:ILE:O	0.62	1.94	7	1
1:A:40:LEU:HD12	1:A:44:THR:CB	0.62	2.24	17	5
1:A:40:LEU:N	1:A:40:LEU:CD1	0.62	2.62	15	1
1:A:70:ILE:HD12	1:A:99:PHE:HD2	0.62	1.51	24	10
1:A:40:LEU:HD23	1:A:44:THR:CG2	0.62	2.24	23	6
1:A:113:SER:HG	1:A:116:HIS:CE1	0.62	2.12	23	10
1:A:102:ARG:HH21	1:A:112:ILE:HD12	0.62	1.54	25	4
1:A:139:TYR:CE2	2:A:178:NTS:O61	0.62	2.52	10	3
1:A:39:ILE:HG23	1:A:75:THR:HG21	0.62	1.71	25	1
1:A:87:LEU:HD11	1:A:123:VAL:HG23	0.62	1.72	22	4
1:A:40:LEU:HD23	1:A:44:THR:HG22	0.62	1.71	5	6
1:A:40:LEU:HD12	1:A:44:THR:HG22	0.62	1.71	4	10
1:A:124:GLY:C	1:A:125:LEU:HD12	0.61	2.19	11	1
1:A:36:PHE:CE2	1:A:51:ARG:CG	0.61	2.82	18	3
1:A:145:LEU:HD13	2:A:178:NTS:O61	0.61	1.95	9	1
1:A:104:GLU:OE2	1:A:145:LEU:HD13	0.61	1.95	24	1
1:A:39:ILE:HG21	1:A:72:SER:HB2	0.61	1.72	2	3
1:A:132:LYS:HB3	1:A:137:THR:HG23	0.61	1.70	11	1
1:A:113:SER:OG	1:A:116:HIS:CE1	0.61	2.54	7	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:GLN:NE2	1:A:54:GLN:H	0.61	1.93	25	4
1:A:71:LYS:CG	1:A:78:TYR:CE2	0.61	2.83	15	2
1:A:69:TYR:CE2	1:A:98:LEU:HD21	0.61	2.31	12	1
1:A:139:TYR:CE2	2:A:178:NTS:O62	0.61	2.54	13	1
1:A:100:LEU:HD13	1:A:117:ALA:CB	0.61	2.24	23	5
1:A:103:LEU:HD21	1:A:106:ASN:HA	0.61	1.71	10	2
1:A:79:LEU:CD1	1:A:87:LEU:HD23	0.61	2.25	1	1
1:A:57:GLN:O	1:A:58:LEU:HD23	0.61	1.96	17	1
1:A:36:PHE:CE2	1:A:51:ARG:CD	0.60	2.83	11	6
1:A:37:LEU:CD1	1:A:146:PHE:CE2	0.60	2.84	14	4
1:A:112:ILE:CG2	1:A:117:ALA:HB1	0.60	2.25	22	7
1:A:55:HIS:CG	1:A:74:GLU:CD	0.60	2.79	12	1
1:A:28:LEU:HD22	1:A:146:PHE:CD1	0.60	2.30	24	3
1:A:82:ASP:OD1	1:A:88:TYR:CE2	0.60	2.54	5	6
1:A:121:TRP:CD1	1:A:134:GLY:C	0.60	2.80	14	9
1:A:69:TYR:CE2	1:A:97:CYS:SG	0.60	2.94	19	2
1:A:88:TYR:CD2	1:A:89:GLY:O	0.60	2.55	1	6
1:A:123:VAL:HG22	1:A:123:VAL:O	0.60	1.96	3	15
1:A:106:ASN:O	1:A:107:HIS:CG	0.60	2.55	4	23
1:A:30:CYS:SG	1:A:146:PHE:CE1	0.60	2.90	22	6
1:A:41:PRO:HD3	1:A:55:HIS:CD2	0.60	2.32	10	2
1:A:144:ILE:HD11	2:A:178:NTS:O61	0.60	1.96	26	2
1:A:83:THR:O	1:A:121:TRP:CH2	0.60	2.55	23	6
1:A:39:ILE:HD11	1:A:79:LEU:CD1	0.60	2.27	11	1
1:A:39:ILE:CD1	1:A:79:LEU:CD2	0.60	2.79	25	2
1:A:82:ASP:OD1	1:A:88:TYR:CD2	0.60	2.54	3	8
1:A:122:PHE:CD2	1:A:144:ILE:HD12	0.60	2.31	17	6
1:A:27:LEU:HD13	1:A:36:PHE:CD1	0.60	2.31	26	1
1:A:82:ASP:CG	1:A:88:TYR:CD1	0.59	2.80	26	10
1:A:115:LYS:O	1:A:116:HIS:CD2	0.59	2.55	3	2
1:A:55:HIS:CE1	1:A:74:GLU:OE1	0.59	2.55	22	2
1:A:79:LEU:HD13	1:A:80:ALA:H	0.59	1.56	25	1
1:A:82:ASP:OD1	1:A:88:TYR:CE1	0.59	2.54	6	11
1:A:60:LEU:HD21	1:A:111:TYR:CZ	0.59	2.32	18	2
1:A:27:LEU:HD11	1:A:149:LEU:HD21	0.59	1.74	12	1
1:A:60:LEU:HD23	1:A:70:ILE:CG1	0.59	2.27	21	2
1:A:83:THR:HG23	1:A:115:LYS:HE2	0.59	1.74	13	1
1:A:139:TYR:CG	2:A:178:NTS:O62	0.59	2.55	21	4
1:A:39:ILE:HD13	1:A:72:SER:HB2	0.59	1.74	24	3
1:A:104:GLU:OE1	1:A:145:LEU:HD11	0.59	1.98	17	1
1:A:145:LEU:HD11	2:A:178:NTS:C6	0.59	2.28	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:LEU:HD11	2:A:178:NTS:C7	0.59	2.27	21	2
1:A:29:TYR:CD1	1:A:36:PHE:CE2	0.59	2.90	7	4
1:A:100:LEU:HD12	1:A:114:LYS:HG2	0.59	1.72	9	8
1:A:72:SER:O	1:A:74:GLU:N	0.59	2.36	16	16
1:A:55:HIS:CD2	1:A:74:GLU:CD	0.59	2.81	12	1
1:A:40:LEU:CD1	1:A:55:HIS:CE1	0.59	2.86	15	1
1:A:40:LEU:HD22	1:A:44:THR:O	0.59	1.98	15	1
1:A:138:HIS:C	2:A:178:NTS:O61	0.59	2.45	24	1
1:A:38:ARG:HB2	1:A:56:ILE:HG22	0.58	1.74	25	1
1:A:81:MET:O	1:A:116:HIS:CE1	0.58	2.56	25	5
1:A:28:LEU:HD21	1:A:146:PHE:CB	0.58	2.26	6	3
1:A:81:MET:HE3	1:A:87:LEU:HD12	0.58	1.74	9	2
1:A:37:LEU:HD11	1:A:146:PHE:CE2	0.58	2.32	14	2
1:A:67:GLU:HG2	1:A:98:LEU:HD13	0.58	1.76	26	7
1:A:53:ASP:CB	1:A:56:ILE:CG2	0.58	2.81	10	9
1:A:108:TYR:CD2	1:A:145:LEU:CD2	0.58	2.87	17	1
1:A:39:ILE:HD13	1:A:40:LEU:N	0.58	2.13	5	2
1:A:37:LEU:HB3	1:A:58:LEU:HD11	0.58	1.76	20	8
1:A:36:PHE:O	1:A:37:LEU:C	0.58	2.46	14	24
1:A:108:TYR:CG	1:A:145:LEU:HB3	0.58	2.33	22	8
1:A:123:VAL:O	1:A:146:PHE:CE2	0.58	2.57	2	7
1:A:87:LEU:CD2	1:A:123:VAL:HG23	0.58	2.28	8	5
1:A:73:THR:O	1:A:73:THR:HG22	0.58	1.96	10	1
1:A:112:ILE:HD11	1:A:122:PHE:CD2	0.58	2.34	14	1
1:A:139:TYR:O	1:A:139:TYR:CG	0.58	2.57	9	1
1:A:68:VAL:C	1:A:98:LEU:HD13	0.58	2.22	12	1
1:A:108:TYR:CE2	1:A:145:LEU:CD2	0.58	2.86	17	2
1:A:39:ILE:HD12	1:A:79:LEU:HD13	0.58	1.74	17	2
1:A:86:LEU:HD12	1:A:133:ARG:HD2	0.58	1.74	18	1
1:A:144:ILE:HG23	2:A:178:NTS:O62	0.58	1.98	24	1
1:A:139:TYR:CG	2:A:178:NTS:O63	0.57	2.57	3	2
1:A:30:CYS:SG	1:A:125:LEU:HD13	0.57	2.39	11	1
1:A:37:LEU:HD12	1:A:146:PHE:CE2	0.57	2.33	12	3
1:A:36:PHE:CD2	1:A:51:ARG:CD	0.57	2.88	21	1
1:A:46:ASP:C	1:A:125:LEU:CD2	0.57	2.78	8	9
1:A:53:ASP:HB3	1:A:56:ILE:HG22	0.57	1.76	4	1
1:A:112:ILE:CD1	1:A:122:PHE:CD1	0.57	2.88	6	3
1:A:40:LEU:HD12	1:A:55:HIS:ND1	0.57	2.14	15	1
1:A:122:PHE:CZ	1:A:139:TYR:CE1	0.57	2.92	18	1
1:A:38:ARG:CZ	1:A:53:ASP:CG	0.57	2.78	9	13
1:A:55:HIS:CD2	1:A:74:GLU:OE1	0.57	2.57	25	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLU:CD	1:A:104:GLU:C	0.57	2.73	7	16
1:A:30:CYS:O	1:A:31:SER:C	0.57	2.48	7	5
1:A:125:LEU:N	1:A:125:LEU:CD1	0.57	2.68	11	2
1:A:81:MET:CG	1:A:87:LEU:HD12	0.57	2.30	16	3
1:A:39:ILE:CD1	1:A:79:LEU:CD1	0.57	2.83	14	1
1:A:45:VAL:C	1:A:46:ASP:CG	0.57	2.73	4	26
1:A:66:GLY:CA	1:A:100:LEU:HD23	0.57	2.30	2	1
1:A:36:PHE:CD2	1:A:51:ARG:HG3	0.57	2.35	7	5
1:A:37:LEU:CG	1:A:125:LEU:HD11	0.57	2.30	6	7
1:A:61:SER:CB	1:A:69:TYR:O	0.57	2.53	19	1
1:A:54:GLN:NE2	1:A:55:HIS:CE1	0.57	2.72	24	1
1:A:125:LEU:HD23	1:A:131:CYS:SG	0.57	2.40	25	1
1:A:115:LYS:C	1:A:116:HIS:CG	0.56	2.83	16	14
1:A:123:VAL:HG13	1:A:123:VAL:O	0.56	2.00	8	5
1:A:30:CYS:SG	1:A:146:PHE:CD1	0.56	2.94	26	1
1:A:67:GLU:CD	1:A:114:LYS:CE	0.56	2.78	24	18
1:A:39:ILE:HG21	1:A:72:SER:OG	0.56	1.99	2	6
1:A:88:TYR:CE2	1:A:89:GLY:O	0.56	2.58	5	5
1:A:112:ILE:CG2	1:A:117:ALA:CB	0.56	2.84	25	13
1:A:80:ALA:CB	1:A:88:TYR:CE1	0.56	2.87	15	4
1:A:40:LEU:HD23	1:A:44:THR:CB	0.56	2.31	23	5
1:A:60:LEU:HD23	1:A:70:ILE:HG23	0.56	1.78	19	1
1:A:104:GLU:HB2	1:A:110:THR:HG21	0.56	1.78	24	2
1:A:62:ALA:HA	1:A:68:VAL:HG12	0.56	1.77	2	12
1:A:29:TYR:HB2	1:A:36:PHE:CD2	0.56	2.35	6	6
1:A:139:TYR:CZ	2:A:178:NTS:O61	0.56	2.59	19	2
1:A:26:LYS:CG	1:A:58:LEU:O	0.56	2.53	12	11
1:A:80:ALA:HB2	1:A:97:CYS:HA	0.56	1.78	26	14
1:A:27:LEU:C	1:A:27:LEU:CD1	0.56	2.77	7	8
1:A:36:PHE:CE2	1:A:51:ARG:HD2	0.56	2.36	11	7
1:A:37:LEU:CD2	1:A:125:LEU:HD11	0.56	2.30	6	2
1:A:54:GLN:CD	1:A:55:HIS:N	0.56	2.64	22	3
1:A:150:PRO:C	1:A:151:VAL:HG22	0.56	2.24	13	7
1:A:112:ILE:O	1:A:113:SER:C	0.56	2.49	12	19
1:A:36:PHE:CE2	1:A:51:ARG:HG3	0.56	2.35	18	4
1:A:31:SER:HB2	1:A:108:TYR:CE1	0.56	2.36	7	5
1:A:104:GLU:OE1	1:A:145:LEU:HD22	0.56	2.01	16	1
1:A:60:LEU:CD2	1:A:111:TYR:OH	0.56	2.53	11	13
1:A:54:GLN:O	1:A:55:HIS:CG	0.56	2.59	26	4
1:A:77:GLN:C	1:A:78:TYR:CD1	0.56	2.84	15	2
1:A:55:HIS:CE1	1:A:74:GLU:OE2	0.56	2.59	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:H	1:A:60:LEU:HD12	0.56	1.61	1	2
1:A:119:LYS:CD	1:A:121:TRP:CZ2	0.56	2.89	16	11
1:A:39:ILE:O	1:A:39:ILE:CG2	0.55	2.54	26	9
1:A:67:GLU:CD	1:A:98:LEU:HD13	0.55	2.26	7	1
1:A:83:THR:HG23	1:A:115:LYS:NZ	0.55	2.16	24	1
1:A:102:ARG:O	1:A:104:GLU:N	0.55	2.39	3	14
1:A:40:LEU:CD1	1:A:44:THR:HG22	0.55	2.31	4	10
1:A:29:TYR:HB2	1:A:36:PHE:CE2	0.55	2.35	19	8
1:A:85:GLY:CA	1:A:121:TRP:CE3	0.55	2.89	13	3
1:A:139:TYR:CZ	2:A:178:NTS:O62	0.55	2.59	13	1
1:A:68:VAL:HG13	1:A:101:GLU:HB2	0.55	1.77	21	2
1:A:72:SER:O	1:A:73:THR:C	0.55	2.48	23	7
1:A:82:ASP:OD1	1:A:88:TYR:CZ	0.55	2.59	1	12
1:A:127:LYS:O	1:A:127:LYS:CD	0.55	2.54	18	15
1:A:35:HIS:CD2	1:A:129:GLY:HA2	0.55	2.37	19	13
1:A:82:ASP:OD2	1:A:88:TYR:CG	0.55	2.60	24	6
1:A:133:ARG:O	1:A:137:THR:HG23	0.55	2.02	22	2
1:A:45:VAL:CG2	1:A:46:ASP:N	0.55	2.69	16	8
1:A:147:LEU:HD23	1:A:148:PRO:N	0.55	2.17	9	1
1:A:144:ILE:HG23	2:A:178:NTS:S6	0.55	2.41	24	1
1:A:68:VAL:HG11	1:A:101:GLU:CD	0.55	2.26	16	2
1:A:37:LEU:HD23	1:A:46:ASP:O	0.55	2.01	13	3
1:A:122:PHE:HB3	1:A:144:ILE:HG22	0.55	1.79	7	4
1:A:79:LEU:HG	1:A:87:LEU:HD23	0.55	1.78	5	1
1:A:29:TYR:CD2	1:A:30:CYS:O	0.55	2.60	14	5
1:A:29:TYR:CE1	1:A:36:PHE:CE1	0.55	2.95	7	4
1:A:36:PHE:CZ	1:A:51:ARG:NH1	0.55	2.75	26	1
1:A:36:PHE:CE2	1:A:51:ARG:HD3	0.54	2.37	21	8
1:A:54:GLN:NE2	1:A:55:HIS:H	0.54	2.00	6	3
1:A:81:MET:SD	1:A:87:LEU:HD12	0.54	2.42	19	5
1:A:82:ASP:OD1	1:A:88:TYR:CG	0.54	2.59	25	4
1:A:120:ASN:O	1:A:122:PHE:CD1	0.54	2.60	21	2
1:A:83:THR:HG23	1:A:115:LYS:CE	0.54	2.32	13	1
1:A:100:LEU:CD1	1:A:117:ALA:CB	0.54	2.86	23	4
1:A:122:PHE:CE1	1:A:144:ILE:HD12	0.54	2.37	5	3
1:A:132:LYS:CB	1:A:137:THR:HG23	0.54	2.33	5	2
1:A:99:PHE:CZ	1:A:123:VAL:CG2	0.54	2.90	18	4
1:A:138:HIS:C	2:A:178:NTS:O63	0.54	2.51	1	1
1:A:30:CYS:O	1:A:31:SER:O	0.54	2.26	7	5
1:A:82:ASP:OD2	1:A:88:TYR:CD1	0.54	2.61	6	1
1:A:71:LYS:HZ3	1:A:76:GLY:HA2	0.54	1.61	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:SER:O	1:A:67:GLU:O	0.54	2.25	1	24
1:A:82:ASP:CG	1:A:88:TYR:CG	0.54	2.86	25	6
1:A:56:ILE:C	1:A:56:ILE:CD1	0.54	2.78	7	6
1:A:99:PHE:CZ	1:A:123:VAL:HG21	0.54	2.37	18	2
1:A:69:TYR:CE1	1:A:98:LEU:CG	0.54	2.91	19	1
1:A:137:THR:O	1:A:138:HIS:CG	0.54	2.61	17	1
1:A:66:GLY:O	1:A:100:LEU:HD23	0.54	2.03	22	10
1:A:31:SER:OG	1:A:108:TYR:CZ	0.54	2.58	12	3
1:A:73:THR:O	1:A:73:THR:CG2	0.54	2.56	10	15
1:A:149:LEU:N	1:A:150:PRO:HD3	0.54	2.17	12	1
1:A:121:TRP:CE2	1:A:134:GLY:C	0.54	2.86	24	2
1:A:36:PHE:CZ	1:A:51:ARG:HD3	0.53	2.38	26	3
1:A:147:LEU:HD23	1:A:147:LEU:C	0.53	2.29	9	1
1:A:36:PHE:CD2	1:A:51:ARG:HD2	0.53	2.38	21	11
1:A:115:LYS:HE2	1:A:116:HIS:CD2	0.53	2.38	2	2
1:A:26:LYS:CE	1:A:27:LEU:N	0.53	2.71	20	4
1:A:81:MET:HE2	1:A:87:LEU:HD11	0.53	1.81	23	1
1:A:93:PRO:C	1:A:94:ASN:ND2	0.53	2.66	3	21
1:A:122:PHE:O	1:A:137:THR:CG2	0.53	2.57	23	5
1:A:138:HIS:O	2:A:178:NTS:S6	0.53	2.67	2	7
1:A:75:THR:O	1:A:76:GLY:C	0.53	2.51	23	9
1:A:27:LEU:O	1:A:27:LEU:CD1	0.53	2.55	18	7
1:A:69:TYR:CE1	1:A:98:LEU:HG	0.53	2.39	19	10
1:A:115:LYS:HE3	1:A:116:HIS:CD2	0.53	2.38	2	4
1:A:54:GLN:HG3	1:A:55:HIS:CE1	0.53	2.38	19	3
1:A:60:LEU:HD12	1:A:60:LEU:N	0.53	2.18	11	1
1:A:123:VAL:O	1:A:144:ILE:HG22	0.53	2.03	24	1
1:A:60:LEU:HD21	1:A:111:TYR:OH	0.53	2.04	9	2
1:A:112:ILE:HD12	1:A:122:PHE:CD1	0.53	2.38	9	1
1:A:50:ASP:O	1:A:52:SER:N	0.53	2.42	15	6
1:A:104:GLU:CG	1:A:145:LEU:HD22	0.53	2.34	11	2
1:A:36:PHE:CE1	1:A:51:ARG:HD3	0.53	2.39	26	1
1:A:104:GLU:CB	1:A:110:THR:OG1	0.53	2.57	18	2
1:A:63:GLU:O	1:A:64:SER:CB	0.53	2.56	11	19
1:A:111:TYR:O	1:A:112:ILE:CG1	0.53	2.57	8	4
1:A:139:TYR:HA	1:A:144:ILE:HD13	0.53	1.81	9	3
1:A:148:PRO:C	1:A:150:PRO:HD3	0.53	2.29	12	2
1:A:104:GLU:OE1	1:A:105:GLU:CG	0.52	2.57	19	4
1:A:127:LYS:O	1:A:127:LYS:CE	0.52	2.57	21	2
1:A:40:LEU:HD12	1:A:44:THR:CG2	0.52	2.34	4	7
1:A:41:PRO:HD3	1:A:55:HIS:CE1	0.52	2.39	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:CG2	1:A:39:ILE:O	0.52	2.58	16	3
1:A:119:LYS:HD2	1:A:121:TRP:CZ2	0.52	2.39	17	12
1:A:57:GLN:C	1:A:58:LEU:HD12	0.52	2.29	8	1
1:A:92:THR:C	1:A:94:ASN:ND2	0.52	2.67	15	13
1:A:108:TYR:CD2	1:A:145:LEU:HG	0.52	2.39	24	3
1:A:71:LYS:CE	1:A:72:SER:O	0.52	2.57	16	1
1:A:104:GLU:CB	1:A:110:THR:HG21	0.52	2.34	24	2
1:A:53:ASP:O	1:A:56:ILE:HG23	0.52	2.05	4	1
1:A:69:TYR:CE1	1:A:98:LEU:CD2	0.52	2.92	12	2
1:A:39:ILE:HD13	1:A:79:LEU:CD2	0.52	2.35	12	1
1:A:86:LEU:HD12	1:A:133:ARG:CD	0.52	2.33	1	2
1:A:53:ASP:CB	1:A:56:ILE:HG22	0.52	2.35	4	1
1:A:27:LEU:HD21	1:A:51:ARG:NE	0.52	2.19	14	1
1:A:66:GLY:O	1:A:100:LEU:CD2	0.52	2.58	8	10
1:A:69:TYR:O	1:A:70:ILE:CG1	0.52	2.57	4	4
1:A:39:ILE:HD13	1:A:40:LEU:H	0.52	1.64	5	1
1:A:108:TYR:CE2	1:A:145:LEU:HD21	0.52	2.39	12	1
1:A:99:PHE:CZ	1:A:123:VAL:HB	0.52	2.40	8	16
1:A:144:ILE:O	1:A:146:PHE:N	0.52	2.43	24	5
1:A:67:GLU:CG	1:A:98:LEU:HD22	0.52	2.35	17	3
1:A:85:GLY:HA3	1:A:121:TRP:CE3	0.52	2.40	13	2
1:A:60:LEU:CD2	1:A:111:TYR:CZ	0.52	2.92	18	3
1:A:38:ARG:CZ	1:A:48:THR:OG1	0.52	2.58	21	14
1:A:86:LEU:HD23	1:A:87:LEU:N	0.52	2.20	11	2
1:A:61:SER:N	1:A:69:TYR:O	0.51	2.43	19	8
1:A:102:ARG:NH2	1:A:112:ILE:CD1	0.51	2.70	22	5
1:A:71:LYS:HG3	1:A:78:TYR:CE2	0.51	2.40	15	9
1:A:87:LEU:CD1	1:A:123:VAL:HG23	0.51	2.34	5	1
1:A:145:LEU:CD1	2:A:178:NTS:O61	0.51	2.58	9	1
1:A:104:GLU:CD	1:A:145:LEU:CD2	0.51	2.83	13	4
1:A:39:ILE:C	1:A:40:LEU:CD1	0.51	2.83	15	1
1:A:101:GLU:O	1:A:102:ARG:CG	0.51	2.58	16	1
1:A:73:THR:CG2	1:A:73:THR:O	0.51	2.59	1	3
1:A:26:LYS:NZ	1:A:58:LEU:C	0.51	2.68	8	1
1:A:116:HIS:CE1	1:A:121:TRP:CH2	0.51	2.98	24	3
1:A:109:ASN:HB3	1:A:111:TYR:CE2	0.51	2.40	18	3
1:A:71:LYS:CE	1:A:71:LYS:C	0.51	2.83	25	1
1:A:38:ARG:NH2	1:A:53:ASP:CG	0.51	2.69	7	8
1:A:134:GLY:N	1:A:135:PRO:CD	0.51	2.74	3	6
1:A:73:THR:O	1:A:74:GLU:CB	0.51	2.58	10	8
1:A:54:GLN:OE1	1:A:54:GLN:N	0.51	2.43	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:PHE:CZ	1:A:51:ARG:HG3	0.51	2.41	18	2
1:A:137:THR:HG23	1:A:137:THR:O	0.51	2.06	12	2
1:A:101:GLU:CD	1:A:102:ARG:N	0.51	2.68	24	1
1:A:108:TYR:CD2	1:A:145:LEU:HB3	0.51	2.41	11	8
1:A:109:ASN:O	1:A:111:TYR:CZ	0.51	2.64	12	4
1:A:82:ASP:OD1	1:A:88:TYR:CD1	0.51	2.64	25	3
1:A:26:LYS:CE	1:A:58:LEU:O	0.51	2.58	16	3
1:A:36:PHE:CZ	1:A:51:ARG:NE	0.51	2.78	17	1
1:A:26:LYS:NZ	1:A:27:LEU:C	0.51	2.69	10	2
1:A:45:VAL:CG1	1:A:87:LEU:O	0.51	2.59	6	7
1:A:99:PHE:CE2	1:A:123:VAL:HG21	0.51	2.41	18	2
1:A:83:THR:HG23	1:A:116:HIS:NE2	0.51	2.21	3	1
1:A:40:LEU:HD23	1:A:44:THR:HB	0.51	1.80	23	4
1:A:31:SER:OG	1:A:145:LEU:CB	0.51	2.59	21	1
1:A:103:LEU:HD21	1:A:105:GLU:O	0.51	2.05	24	1
1:A:39:ILE:HD12	1:A:77:GLN:CG	0.51	2.35	26	1
1:A:31:SER:CB	1:A:108:TYR:CE1	0.51	2.94	7	2
1:A:56:ILE:C	1:A:56:ILE:HD13	0.51	2.31	15	9
1:A:36:PHE:CD2	1:A:51:ARG:HD3	0.51	2.41	6	4
1:A:135:PRO:O	1:A:136:ARG:CG	0.51	2.59	2	14
1:A:103:LEU:HD21	1:A:107:HIS:N	0.51	2.20	26	3
1:A:104:GLU:CD	1:A:105:GLU:N	0.51	2.69	4	4
1:A:127:LYS:CE	2:A:178:NTS:O11	0.51	2.59	11	2
1:A:27:LEU:CD1	1:A:28:LEU:O	0.51	2.58	21	3
1:A:68:VAL:HG21	1:A:111:TYR:CD2	0.51	2.41	11	1
1:A:135:PRO:O	1:A:136:ARG:CD	0.51	2.59	19	2
1:A:81:MET:CE	1:A:87:LEU:HD12	0.50	2.35	1	1
1:A:121:TRP:NE1	1:A:134:GLY:C	0.50	2.69	7	8
1:A:139:TYR:C	2:A:178:NTS:O63	0.50	2.54	9	4
1:A:85:GLY:CA	1:A:121:TRP:CZ3	0.50	2.95	13	2
1:A:125:LEU:CD2	1:A:131:CYS:SG	0.50	2.99	25	1
1:A:133:ARG:O	1:A:137:THR:CG2	0.50	2.60	22	2
1:A:108:TYR:CE2	1:A:145:LEU:CG	0.50	2.93	12	1
1:A:149:LEU:O	1:A:149:LEU:CG	0.50	2.59	12	1
1:A:104:GLU:OE1	1:A:145:LEU:CD2	0.50	2.60	19	2
1:A:53:ASP:CG	1:A:54:GLN:NE2	0.50	2.69	21	2
1:A:64:SER:O	1:A:65:VAL:C	0.50	2.54	12	13
1:A:127:LYS:CE	2:A:178:NTS:O13	0.50	2.59	23	3
1:A:103:LEU:CD2	1:A:107:HIS:N	0.50	2.74	26	1
1:A:111:TYR:O	1:A:122:PHE:CD2	0.50	2.64	1	1
1:A:45:VAL:CG2	1:A:87:LEU:O	0.50	2.59	23	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:THR:O	1:A:49:ARG:C	0.50	2.55	25	12
1:A:44:THR:CG2	1:A:45:VAL:N	0.50	2.74	5	7
1:A:54:GLN:O	1:A:55:HIS:CD2	0.50	2.64	13	3
1:A:26:LYS:O	1:A:57:GLN:CB	0.50	2.60	7	2
1:A:68:VAL:HG21	1:A:111:TYR:CD1	0.50	2.42	14	2
1:A:57:GLN:O	1:A:58:LEU:CD2	0.50	2.59	17	1
1:A:39:ILE:CG2	1:A:75:THR:HG21	0.50	2.35	25	1
1:A:26:LYS:O	1:A:57:GLN:CG	0.50	2.59	19	5
1:A:112:ILE:HD11	1:A:120:ASN:CA	0.50	2.37	9	1
1:A:109:ASN:CB	1:A:111:TYR:CZ	0.50	2.94	14	4
1:A:68:VAL:O	1:A:99:PHE:N	0.50	2.44	5	16
1:A:38:ARG:NH2	1:A:48:THR:CG2	0.50	2.74	4	3
1:A:132:LYS:CG	1:A:136:ARG:O	0.50	2.60	9	1
1:A:62:ALA:CA	1:A:68:VAL:HG12	0.50	2.36	19	6
1:A:122:PHE:CD1	1:A:138:HIS:HA	0.50	2.41	3	4
1:A:38:ARG:HH21	1:A:48:THR:HG21	0.50	1.65	4	3
1:A:51:ARG:O	1:A:51:ARG:CG	0.50	2.60	5	5
1:A:80:ALA:HB1	1:A:88:TYR:CE1	0.50	2.42	15	2
1:A:108:TYR:CD1	1:A:147:LEU:HD23	0.50	2.41	18	4
1:A:54:GLN:NE2	1:A:55:HIS:CG	0.50	2.80	15	2
1:A:40:LEU:CD1	1:A:44:THR:O	0.50	2.59	26	4
1:A:96:GLU:OE2	1:A:115:LYS:CD	0.50	2.60	22	1
1:A:83:THR:O	1:A:121:TRP:CZ3	0.50	2.65	23	1
1:A:36:PHE:N	1:A:48:THR:O	0.50	2.45	12	13
1:A:39:ILE:CG2	1:A:72:SER:OG	0.50	2.60	1	6
1:A:105:GLU:CG	1:A:106:ASN:N	0.50	2.75	14	15
1:A:112:ILE:O	1:A:114:LYS:N	0.50	2.45	1	12
1:A:138:HIS:N	1:A:138:HIS:ND1	0.50	2.60	4	3
1:A:26:LYS:HZ2	1:A:59:GLN:N	0.50	2.04	8	1
1:A:81:MET:SD	1:A:87:LEU:CD1	0.50	3.00	16	4
1:A:69:TYR:CD2	1:A:97:CYS:SG	0.50	3.05	19	1
1:A:150:PRO:O	1:A:151:VAL:CG1	0.49	2.60	11	18
1:A:109:ASN:HB3	1:A:111:TYR:CZ	0.49	2.41	14	5
1:A:36:PHE:CE2	1:A:51:ARG:HG2	0.49	2.41	18	1
1:A:81:MET:HE2	1:A:87:LEU:CD1	0.49	2.36	23	1
1:A:41:PRO:CD	1:A:54:GLN:OE1	0.49	2.59	23	2
1:A:27:LEU:O	1:A:27:LEU:CG	0.49	2.60	6	5
1:A:94:ASN:O	1:A:96:GLU:N	0.49	2.46	3	17
1:A:69:TYR:CE1	1:A:98:LEU:HD21	0.49	2.41	2	3
1:A:29:TYR:CE1	1:A:36:PHE:CZ	0.49	3.00	7	2
1:A:69:TYR:CE2	1:A:98:LEU:HG	0.49	2.42	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLU:HG2	1:A:145:LEU:HD11	0.49	1.83	9	1
1:A:68:VAL:HG22	1:A:101:GLU:HB2	0.49	1.82	12	2
1:A:101:GLU:CD	1:A:109:ASN:ND2	0.49	2.70	21	3
1:A:73:THR:O	1:A:73:THR:HG23	0.49	2.07	5	3
1:A:54:GLN:NE2	1:A:55:HIS:N	0.49	2.60	6	2
1:A:27:LEU:O	1:A:149:LEU:CD2	0.49	2.60	9	1
1:A:108:TYR:CE2	1:A:145:LEU:HG	0.49	2.42	12	3
1:A:84:ASP:OD2	1:A:133:ARG:CZ	0.49	2.60	14	1
1:A:56:ILE:O	1:A:58:LEU:CD1	0.49	2.60	18	4
1:A:93:PRO:C	1:A:94:ASN:CG	0.49	2.80	2	7
1:A:107:HIS:HB3	1:A:147:LEU:HD23	0.49	1.83	3	2
1:A:110:THR:HG22	1:A:144:ILE:O	0.49	2.07	12	1
1:A:91:GLN:O	1:A:91:GLN:CG	0.49	2.60	19	3
1:A:38:ARG:NE	1:A:48:THR:OG1	0.49	2.45	2	23
1:A:122:PHE:N	1:A:137:THR:O	0.49	2.46	8	7
1:A:101:GLU:CD	1:A:109:ASN:CG	0.49	2.80	5	2
1:A:94:ASN:O	1:A:95:GLU:C	0.49	2.56	13	10
1:A:38:ARG:HD3	1:A:40:LEU:HD21	0.49	1.83	7	1
1:A:110:THR:CG2	1:A:144:ILE:HG13	0.49	2.37	22	5
1:A:115:LYS:C	1:A:116:HIS:CD2	0.49	2.91	18	2
1:A:56:ILE:O	1:A:56:ILE:CD1	0.49	2.59	24	5
1:A:36:PHE:CD1	1:A:50:ASP:HA	0.49	2.42	10	5
1:A:80:ALA:HB3	1:A:88:TYR:O	0.49	2.07	19	6
1:A:132:LYS:CE	1:A:136:ARG:O	0.49	2.60	11	1
1:A:122:PHE:O	1:A:137:THR:OG1	0.49	2.30	9	3
1:A:35:HIS:NE2	1:A:128:ASN:C	0.49	2.71	16	5
1:A:60:LEU:CD1	1:A:111:TYR:OH	0.49	2.60	24	5
1:A:121:TRP:CE2	1:A:134:GLY:CA	0.49	2.96	13	1
1:A:120:ASN:O	1:A:122:PHE:N	0.49	2.46	18	11
1:A:40:LEU:CD2	1:A:44:THR:HG22	0.49	2.38	23	3
1:A:54:GLN:HE21	1:A:55:HIS:N	0.49	2.06	15	4
1:A:147:LEU:O	1:A:149:LEU:CD2	0.49	2.60	10	3
1:A:27:LEU:HD21	1:A:51:ARG:CZ	0.49	2.37	13	2
1:A:69:TYR:CE1	1:A:98:LEU:HD11	0.49	2.43	19	1
1:A:101:GLU:HG3	1:A:111:TYR:CD2	0.49	2.43	13	8
1:A:145:LEU:N	1:A:145:LEU:CD2	0.49	2.73	5	2
1:A:28:LEU:HD21	1:A:146:PHE:CG	0.49	2.43	6	1
1:A:73:THR:O	1:A:74:GLU:CG	0.49	2.60	10	2
1:A:104:GLU:CD	1:A:105:GLU:CG	0.49	2.86	25	2
1:A:41:PRO:CD	1:A:55:HIS:CE1	0.49	2.96	17	1
1:A:71:LYS:O	1:A:73:THR:N	0.48	2.46	22	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:LYS:O	1:A:138:HIS:CD2	0.48	2.66	1	1
1:A:119:LYS:HB3	1:A:121:TRP:CD1	0.48	2.43	7	20
1:A:39:ILE:CD1	1:A:45:VAL:CG1	0.48	2.85	25	2
1:A:137:THR:C	1:A:138:HIS:ND1	0.48	2.70	25	6
1:A:63:GLU:CG	1:A:98:LEU:HD21	0.48	2.38	9	5
1:A:65:VAL:O	1:A:67:GLU:CD	0.48	2.56	4	4
1:A:44:THR:C	1:A:45:VAL:CG2	0.48	2.86	23	5
1:A:60:LEU:N	1:A:60:LEU:CD1	0.48	2.75	2	2
1:A:139:TYR:HA	1:A:144:ILE:CD1	0.48	2.38	9	1
1:A:27:LEU:CD1	1:A:149:LEU:HD21	0.48	2.37	12	2
1:A:121:TRP:CA	1:A:137:THR:HG23	0.48	2.37	1	2
1:A:104:GLU:OE1	1:A:105:GLU:N	0.48	2.46	6	16
1:A:37:LEU:O	1:A:58:LEU:CD1	0.48	2.61	4	1
1:A:82:ASP:CG	1:A:88:TYR:CE1	0.48	2.91	6	2
1:A:61:SER:O	1:A:62:ALA:C	0.48	2.57	19	24
1:A:113:SER:OG	1:A:116:HIS:ND1	0.48	2.47	12	16
1:A:36:PHE:CG	1:A:51:ARG:HG3	0.48	2.43	18	2
1:A:101:GLU:HG3	1:A:111:TYR:CE2	0.48	2.43	5	10
1:A:86:LEU:O	1:A:87:LEU:C	0.48	2.57	23	23
1:A:51:ARG:NE	1:A:51:ARG:O	0.48	2.46	15	5
1:A:40:LEU:CD2	1:A:53:ASP:OD2	0.48	2.62	6	1
1:A:35:HIS:CE1	1:A:127:LYS:C	0.48	2.92	16	1
1:A:35:HIS:HE2	1:A:129:GLY:CA	0.48	2.22	25	1
1:A:80:ALA:N	1:A:88:TYR:O	0.48	2.47	17	18
1:A:26:LYS:HZ2	1:A:27:LEU:C	0.48	2.17	10	1
1:A:125:LEU:HD23	1:A:125:LEU:N	0.48	2.23	16	1
1:A:31:SER:N	1:A:145:LEU:O	0.48	2.45	21	2
1:A:99:PHE:CE1	1:A:123:VAL:HB	0.48	2.43	12	16
1:A:101:GLU:C	1:A:102:ARG:HG2	0.48	2.33	18	1
1:A:103:LEU:HD23	1:A:108:TYR:O	0.48	2.08	21	1
1:A:104:GLU:CA	1:A:104:GLU:OE1	0.48	2.61	21	1
1:A:71:LYS:HG3	1:A:78:TYR:CE1	0.48	2.44	25	4
1:A:136:ARG:C	1:A:137:THR:CG2	0.48	2.86	21	4
1:A:139:TYR:C	2:A:178:NTS:O62	0.48	2.57	11	2
1:A:58:LEU:CD2	1:A:79:LEU:HD22	0.48	2.38	22	1
1:A:133:ARG:O	1:A:135:PRO:N	0.48	2.47	24	1
1:A:66:GLY:N	1:A:101:GLU:O	0.48	2.47	7	5
1:A:78:TYR:O	1:A:89:GLY:CA	0.48	2.62	12	6
1:A:55:HIS:ND1	1:A:74:GLU:CG	0.48	2.76	12	1
1:A:75:THR:CG2	1:A:77:GLN:OE1	0.48	2.61	18	2
1:A:105:GLU:OE1	1:A:108:TYR:CE2	0.48	2.67	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:LEU:O	1:A:149:LEU:CD1	0.47	2.61	12	5
1:A:71:LYS:HG2	1:A:78:TYR:CD2	0.47	2.44	15	1
1:A:133:ARG:O	1:A:136:ARG:N	0.47	2.47	24	1
1:A:51:ARG:N	1:A:51:ARG:HD3	0.47	2.24	7	5
1:A:112:ILE:CD1	1:A:122:PHE:CZ	0.47	2.96	3	5
1:A:81:MET:CE	1:A:122:PHE:O	0.47	2.60	17	4
1:A:104:GLU:OE1	1:A:145:LEU:CD1	0.47	2.62	17	2
1:A:88:TYR:HH	1:A:96:GLU:CD	0.47	2.17	14	4
1:A:109:ASN:HB3	1:A:111:TYR:CE1	0.47	2.44	14	1
1:A:104:GLU:OE1	1:A:145:LEU:HD13	0.47	2.10	16	1
1:A:133:ARG:CG	1:A:133:ARG:O	0.47	2.62	17	1
1:A:53:ASP:HB3	1:A:56:ILE:CG2	0.47	2.39	10	8
1:A:112:ILE:HG13	1:A:122:PHE:CD2	0.47	2.44	3	1
1:A:78:TYR:N	1:A:78:TYR:CD1	0.47	2.83	8	2
1:A:100:LEU:HD13	1:A:117:ALA:HB1	0.47	1.86	8	2
1:A:59:GLN:CB	1:A:73:THR:HG23	0.47	2.39	25	3
1:A:113:SER:O	1:A:117:ALA:N	0.47	2.48	24	6
1:A:75:THR:O	1:A:77:GLN:N	0.47	2.48	12	1
1:A:36:PHE:CD1	1:A:51:ARG:HD3	0.47	2.44	26	1
1:A:108:TYR:O	1:A:109:ASN:CG	0.47	2.58	1	4
1:A:27:LEU:HD21	1:A:149:LEU:HD11	0.47	1.87	5	1
1:A:71:LYS:NZ	1:A:72:SER:C	0.47	2.73	6	2
1:A:94:ASN:C	1:A:96:GLU:N	0.47	2.71	7	6
1:A:99:PHE:O	1:A:101:GLU:N	0.47	2.47	17	4
1:A:104:GLU:OE1	1:A:105:GLU:CB	0.47	2.62	19	7
1:A:108:TYR:CD2	1:A:145:LEU:CG	0.47	2.98	12	2
1:A:84:ASP:O	1:A:134:GLY:N	0.47	2.48	17	2
1:A:55:HIS:CE1	1:A:74:GLU:HG2	0.47	2.44	23	1
1:A:41:PRO:HG3	1:A:55:HIS:CD2	0.47	2.43	4	1
1:A:111:TYR:CD1	1:A:111:TYR:N	0.47	2.82	4	3
1:A:111:TYR:CD1	1:A:123:VAL:HG11	0.47	2.44	7	1
1:A:26:LYS:CD	1:A:26:LYS:C	0.47	2.88	8	1
1:A:147:LEU:HD23	1:A:148:PRO:HD2	0.47	1.87	13	1
1:A:78:TYR:CD1	1:A:78:TYR:N	0.47	2.83	15	1
1:A:121:TRP:NE1	1:A:134:GLY:O	0.47	2.48	24	5
1:A:72:SER:N	1:A:77:GLN:O	0.47	2.48	5	4
1:A:84:ASP:C	1:A:86:LEU:N	0.47	2.72	17	6
1:A:83:THR:CG2	1:A:115:LYS:CE	0.47	2.93	13	1
1:A:71:LYS:HG3	1:A:78:TYR:CZ	0.47	2.45	15	19
1:A:104:GLU:CG	1:A:145:LEU:HD21	0.47	2.40	19	2
1:A:82:ASP:O	1:A:116:HIS:NE2	0.46	2.47	25	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLU:HG3	1:A:145:LEU:HD21	0.46	1.86	6	2
1:A:26:LYS:NZ	1:A:58:LEU:O	0.46	2.48	16	4
1:A:53:ASP:HB3	1:A:56:ILE:HG23	0.46	1.86	19	2
1:A:96:GLU:CD	1:A:115:LYS:HZ3	0.46	2.19	3	1
1:A:63:GLU:HG2	1:A:69:TYR:CE2	0.46	2.45	4	2
1:A:53:ASP:HB2	1:A:56:ILE:CG2	0.46	2.41	15	6
1:A:75:THR:O	1:A:75:THR:HG23	0.46	2.09	26	1
1:A:94:ASN:O	1:A:98:LEU:HD23	0.46	2.11	4	2
1:A:36:PHE:CE1	1:A:50:ASP:HA	0.46	2.46	17	5
1:A:38:ARG:CB	1:A:56:ILE:HG22	0.46	2.40	25	3
1:A:78:TYR:O	1:A:79:LEU:C	0.46	2.58	13	5
1:A:36:PHE:CE1	1:A:51:ARG:CD	0.46	2.97	26	1
1:A:121:TRP:CH2	1:A:134:GLY:HA2	0.46	2.45	8	2
1:A:93:PRO:O	1:A:94:ASN:CG	0.46	2.59	2	1
1:A:111:TYR:CD1	1:A:123:VAL:CG1	0.46	2.99	7	2
1:A:71:LYS:CD	1:A:77:GLN:O	0.46	2.63	8	1
1:A:139:TYR:C	2:A:178:NTS:O61	0.46	2.59	4	1
1:A:36:PHE:CD2	1:A:51:ARG:HB3	0.46	2.46	5	1
1:A:29:TYR:CE1	1:A:30:CYS:O	0.46	2.69	12	3
1:A:108:TYR:CG	1:A:145:LEU:CB	0.46	2.98	11	2
1:A:88:TYR:CE2	1:A:90:SER:HB2	0.46	2.46	18	1
1:A:122:PHE:N	1:A:137:THR:OG1	0.46	2.49	22	6
1:A:101:GLU:OE2	1:A:109:ASN:CG	0.46	2.59	5	3
1:A:78:TYR:CD1	1:A:93:PRO:HB3	0.46	2.46	22	2
1:A:126:LYS:CD	1:A:128:ASN:OD1	0.46	2.64	22	1
1:A:36:PHE:CZ	1:A:51:ARG:CD	0.46	2.99	26	1
1:A:70:ILE:HG22	1:A:79:LEU:HB2	0.46	1.88	25	4
1:A:74:GLU:CG	1:A:75:THR:N	0.46	2.79	3	1
1:A:121:TRP:CE2	1:A:134:GLY:HA3	0.46	2.46	7	4
1:A:63:GLU:HG2	1:A:69:TYR:CD2	0.46	2.45	4	2
1:A:104:GLU:CG	1:A:145:LEU:HD11	0.46	2.41	9	1
1:A:71:LYS:NZ	1:A:77:GLN:O	0.46	2.49	24	2
1:A:53:ASP:CG	1:A:54:GLN:OE1	0.46	2.59	13	4
1:A:84:ASP:O	1:A:86:LEU:N	0.46	2.49	17	1
1:A:87:LEU:HD12	1:A:87:LEU:H	0.46	1.69	17	1
1:A:57:GLN:NE2	1:A:74:GLU:CD	0.46	2.74	24	1
1:A:46:ASP:OD1	1:A:46:ASP:N	0.46	2.47	11	9
1:A:31:SER:HB2	1:A:108:TYR:CD1	0.46	2.46	14	3
1:A:36:PHE:CD1	1:A:51:ARG:HG3	0.46	2.46	18	2
1:A:94:ASN:ND2	1:A:94:ASN:N	0.46	2.64	15	3
1:A:55:HIS:CG	1:A:74:GLU:HG2	0.46	2.46	26	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:PHE:CD1	1:A:144:ILE:HD12	0.46	2.46	5	2
1:A:104:GLU:OE1	1:A:145:LEU:CG	0.46	2.64	17	1
1:A:108:TYR:CZ	1:A:145:LEU:HD23	0.46	2.45	17	1
1:A:86:LEU:HD12	1:A:133:ARG:HB3	0.46	1.87	18	1
1:A:108:TYR:CE2	1:A:145:LEU:CD1	0.46	2.97	20	2
1:A:104:GLU:CD	1:A:104:GLU:O	0.46	2.59	7	2
1:A:54:GLN:HE22	1:A:55:HIS:CD2	0.46	2.28	15	2
1:A:40:LEU:O	1:A:77:GLN:NE2	0.45	2.50	9	3
1:A:28:LEU:CD2	1:A:146:PHE:CD1	0.45	2.98	11	2
1:A:121:TRP:CD2	1:A:134:GLY:HA3	0.45	2.46	15	1
1:A:51:ARG:O	1:A:51:ARG:CD	0.45	2.64	15	3
1:A:71:LYS:HG3	1:A:78:TYR:CD2	0.45	2.46	4	1
1:A:149:LEU:N	1:A:150:PRO:CD	0.45	2.79	12	1
1:A:56:ILE:O	1:A:56:ILE:HG12	0.45	2.12	14	1
1:A:104:GLU:HB2	1:A:110:THR:CG2	0.45	2.41	23	3
1:A:37:LEU:CD1	1:A:125:LEU:HD11	0.45	2.41	26	1
1:A:67:GLU:C	1:A:98:LEU:CD2	0.45	2.90	5	1
1:A:109:ASN:O	1:A:110:THR:C	0.45	2.58	7	3
1:A:57:GLN:OE1	1:A:74:GLU:CG	0.45	2.64	14	1
1:A:84:ASP:O	1:A:133:ARG:C	0.45	2.60	17	1
1:A:122:PHE:O	1:A:137:THR:HG21	0.45	2.10	20	2
1:A:37:LEU:C	1:A:58:LEU:CD1	0.45	2.90	23	1
1:A:99:PHE:O	1:A:100:LEU:C	0.45	2.59	17	5
1:A:36:PHE:CE1	1:A:51:ARG:HG3	0.45	2.45	18	2
1:A:69:TYR:CZ	1:A:98:LEU:HG	0.45	2.46	20	14
1:A:73:THR:O	1:A:74:GLU:CD	0.45	2.60	8	3
1:A:38:ARG:NH1	1:A:53:ASP:OD1	0.45	2.49	17	1
1:A:112:ILE:O	1:A:112:ILE:HG22	0.45	2.12	18	2
1:A:119:LYS:HD3	1:A:121:TRP:CZ2	0.45	2.45	23	1
1:A:138:HIS:O	1:A:139:TYR:O	0.45	2.34	21	15
1:A:115:LYS:HB3	1:A:116:HIS:CE1	0.45	2.46	2	1
1:A:48:THR:O	1:A:50:ASP:N	0.45	2.50	4	1
1:A:75:THR:OG1	1:A:76:GLY:N	0.45	2.49	10	5
1:A:38:ARG:NH1	1:A:53:ASP:CG	0.45	2.74	8	2
1:A:75:THR:C	1:A:77:GLN:N	0.45	2.74	12	1
1:A:55:HIS:CE1	1:A:74:GLU:HG3	0.45	2.46	13	1
1:A:39:ILE:O	1:A:54:GLN:NE2	0.45	2.50	14	1
1:A:139:TYR:CA	2:A:178:NTS:O62	0.45	2.64	19	1
1:A:54:GLN:OE1	1:A:55:HIS:N	0.45	2.42	24	1
1:A:108:TYR:CG	1:A:145:LEU:HG	0.45	2.46	24	1
1:A:52:SER:O	1:A:52:SER:OG	0.45	2.32	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:HG11	1:A:101:GLU:OE2	0.45	2.11	10	1
1:A:53:ASP:OD2	1:A:54:GLN:NE2	0.45	2.50	21	2
1:A:37:LEU:CG	1:A:125:LEU:HD21	0.45	2.42	10	2
1:A:111:TYR:O	1:A:122:PHE:CD1	0.45	2.69	7	1
1:A:81:MET:CE	1:A:137:THR:HG21	0.45	2.42	8	1
1:A:121:TRP:CD2	1:A:134:GLY:CA	0.45	3.00	13	1
1:A:112:ILE:CD1	1:A:122:PHE:CE2	0.45	2.90	14	1
1:A:57:GLN:N	1:A:57:GLN:OE1	0.45	2.50	18	2
1:A:54:GLN:CG	1:A:55:HIS:CE1	0.45	2.99	19	1
1:A:71:LYS:HZ2	1:A:76:GLY:HA2	0.45	1.72	25	1
1:A:135:PRO:O	1:A:136:ARG:NE	0.45	2.50	25	1
1:A:39:ILE:HD12	1:A:77:GLN:HG2	0.45	1.87	26	1
1:A:26:LYS:NZ	1:A:27:LEU:O	0.45	2.49	1	1
1:A:88:TYR:OH	1:A:96:GLU:CD	0.45	2.60	12	8
1:A:120:ASN:O	1:A:137:THR:O	0.45	2.35	4	5
1:A:57:GLN:NE2	1:A:73:THR:O	0.45	2.50	6	1
1:A:94:ASN:N	1:A:97:CYS:SG	0.45	2.89	13	1
1:A:38:ARG:NH1	1:A:53:ASP:OD2	0.45	2.50	21	1
1:A:100:LEU:O	1:A:112:ILE:N	0.45	2.49	23	1
1:A:79:LEU:HD13	1:A:80:ALA:N	0.45	2.27	25	1
1:A:130:SER:O	1:A:131:CYS:C	0.45	2.59	13	4
1:A:35:HIS:NE2	1:A:129:GLY:CA	0.45	2.80	10	2
1:A:94:ASN:O	1:A:97:CYS:N	0.45	2.50	13	4
1:A:111:TYR:HB2	1:A:123:VAL:HG11	0.45	1.89	22	6
1:A:57:GLN:N	1:A:57:GLN:CD	0.45	2.75	25	1
1:A:81:MET:CE	1:A:85:GLY:O	0.45	2.64	1	2
1:A:83:THR:HA	1:A:116:HIS:CD2	0.45	2.47	18	2
1:A:71:LYS:CG	1:A:78:TYR:CD2	0.45	3.00	15	1
1:A:102:ARG:O	1:A:110:THR:OG1	0.45	2.35	16	1
1:A:106:ASN:OD1	1:A:106:ASN:C	0.45	2.60	20	1
1:A:101:GLU:OE2	1:A:102:ARG:C	0.45	2.59	24	1
1:A:57:GLN:CD	1:A:74:GLU:OE1	0.45	2.60	26	1
1:A:92:THR:O	1:A:94:ASN:ND2	0.44	2.50	15	2
1:A:104:GLU:OE1	1:A:104:GLU:C	0.44	2.60	12	2
1:A:26:LYS:CE	1:A:27:LEU:C	0.44	2.91	20	1
1:A:101:GLU:OE2	1:A:103:LEU:N	0.44	2.50	20	1
1:A:132:LYS:HB3	1:A:137:THR:HG22	0.44	1.88	22	1
1:A:54:GLN:NE2	1:A:55:HIS:ND1	0.44	2.64	24	1
1:A:48:THR:C	1:A:50:ASP:N	0.44	2.73	4	8
1:A:38:ARG:NH2	1:A:48:THR:OG1	0.44	2.50	21	3
1:A:39:ILE:O	1:A:39:ILE:HG22	0.44	2.12	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD11	1:A:99:PHE:HZ	0.44	1.72	16	1
1:A:104:GLU:C	1:A:104:GLU:OE2	0.44	2.60	16	1
1:A:106:ASN:O	1:A:106:ASN:CG	0.44	2.60	17	2
1:A:113:SER:N	1:A:121:TRP:O	0.44	2.50	19	3
1:A:139:TYR:N	2:A:178:NTS:O61	0.44	2.50	24	1
1:A:127:LYS:CE	2:A:178:NTS:O33	0.44	2.66	1	1
1:A:101:GLU:OE2	1:A:109:ASN:ND2	0.44	2.50	14	4
1:A:110:THR:HG21	1:A:145:LEU:CD2	0.44	2.42	22	1
1:A:113:SER:O	1:A:116:HIS:C	0.44	2.60	23	1
1:A:104:GLU:HG3	1:A:145:LEU:HD11	0.44	1.90	25	1
1:A:131:CYS:SG	1:A:132:LYS:N	0.44	2.90	16	2
1:A:84:ASP:O	1:A:85:GLY:C	0.44	2.60	17	1
1:A:115:LYS:HD3	1:A:116:HIS:CD2	0.44	2.48	18	1
1:A:45:VAL:O	1:A:46:ASP:CG	0.44	2.61	4	4
1:A:46:ASP:N	1:A:46:ASP:OD1	0.44	2.50	24	4
1:A:132:LYS:NZ	1:A:136:ARG:O	0.44	2.50	11	1
1:A:139:TYR:CD1	2:A:178:NTS:O62	0.44	2.71	19	1
1:A:138:HIS:O	2:A:178:NTS:O63	0.44	2.36	22	1
1:A:26:LYS:NZ	1:A:73:THR:OG1	0.44	2.49	23	1
1:A:108:TYR:C	1:A:109:ASN:OD1	0.44	2.60	1	2
1:A:123:VAL:O	1:A:123:VAL:CG2	0.44	2.65	3	3
1:A:112:ILE:CD1	1:A:120:ASN:HA	0.44	2.42	9	1
1:A:122:PHE:HB3	1:A:144:ILE:CG2	0.44	2.43	18	1
1:A:39:ILE:CG2	1:A:75:THR:CG2	0.44	2.96	19	1
1:A:30:CYS:HA	1:A:145:LEU:O	0.44	2.12	21	1
1:A:26:LYS:CG	1:A:150:PRO:HA	0.44	2.43	23	1
1:A:45:VAL:C	1:A:46:ASP:OD1	0.44	2.60	2	5
1:A:100:LEU:O	1:A:111:TYR:HA	0.44	2.13	17	2
1:A:147:LEU:C	1:A:147:LEU:CD2	0.44	2.91	9	1
1:A:80:ALA:HB3	1:A:88:TYR:CE1	0.44	2.47	10	2
1:A:67:GLU:CG	1:A:98:LEU:HD13	0.44	2.42	26	2
1:A:121:TRP:CD1	1:A:134:GLY:CA	0.44	2.99	14	1
1:A:109:ASN:O	1:A:111:TYR:CG	0.44	2.71	17	3
1:A:27:LEU:HD21	1:A:51:ARG:NH2	0.44	2.28	2	1
1:A:71:LYS:HZ3	1:A:77:GLN:N	0.44	2.10	2	1
1:A:31:SER:HB2	1:A:108:TYR:CZ	0.44	2.48	6	2
1:A:26:LYS:HZ1	1:A:58:LEU:N	0.44	2.10	14	2
1:A:57:GLN:NE2	1:A:74:GLU:OE1	0.44	2.50	8	1
1:A:59:GLN:HB2	1:A:73:THR:CG2	0.44	2.43	11	2
1:A:112:ILE:HG13	1:A:122:PHE:CD1	0.44	2.48	14	1
1:A:62:ALA:HA	1:A:68:VAL:CG1	0.44	2.43	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:GLY:HA2	1:A:101:GLU:O	0.44	2.12	22	2
1:A:54:GLN:CD	1:A:54:GLN:N	0.44	2.74	13	2
1:A:26:LYS:CE	1:A:28:LEU:N	0.43	2.80	6	1
1:A:30:CYS:HB2	1:A:35:HIS:N	0.43	2.28	18	2
1:A:127:LYS:N	1:A:127:LYS:HD2	0.43	2.28	10	8
1:A:68:VAL:CG1	1:A:101:GLU:HB3	0.43	2.44	13	1
1:A:104:GLU:CB	1:A:110:THR:CG2	0.43	2.96	24	2
1:A:102:ARG:N	1:A:102:ARG:CD	0.43	2.81	2	1
1:A:27:LEU:CD2	1:A:149:LEU:HD11	0.43	2.43	5	1
1:A:77:GLN:O	1:A:78:TYR:CD1	0.43	2.71	10	1
1:A:96:GLU:O	1:A:97:CYS:C	0.43	2.60	22	2
1:A:123:VAL:O	1:A:123:VAL:HG13	0.43	2.14	24	1
1:A:35:HIS:CG	1:A:49:ARG:HA	0.43	2.48	14	4
1:A:131:CYS:O	1:A:132:LYS:NZ	0.43	2.50	1	2
1:A:112:ILE:HG23	1:A:117:ALA:CB	0.43	2.44	6	1
1:A:82:ASP:O	1:A:85:GLY:N	0.43	2.49	7	1
1:A:36:PHE:O	1:A:37:LEU:O	0.43	2.35	26	5
1:A:104:GLU:OE2	1:A:105:GLU:CG	0.43	2.67	11	1
1:A:114:LYS:C	1:A:116:HIS:N	0.43	2.73	11	2
1:A:68:VAL:CG1	1:A:101:GLU:CB	0.43	2.95	13	1
1:A:97:CYS:SG	1:A:98:LEU:N	0.43	2.91	13	1
1:A:29:TYR:CD1	1:A:30:CYS:N	0.43	2.86	21	2
1:A:68:VAL:CG1	1:A:101:GLU:HB2	0.43	2.44	21	2
1:A:31:SER:OG	1:A:145:LEU:HB2	0.43	2.12	21	1
1:A:68:VAL:CG2	1:A:111:TYR:CD2	0.43	3.01	26	1
1:A:103:LEU:O	1:A:104:GLU:C	0.43	2.61	6	1
1:A:101:GLU:HB2	1:A:111:TYR:CD2	0.43	2.49	24	1
1:A:127:LYS:N	1:A:127:LYS:CD	0.43	2.78	6	2
1:A:55:HIS:CG	1:A:74:GLU:HG3	0.43	2.49	23	2
1:A:27:LEU:CD2	1:A:51:ARG:CZ	0.43	2.96	24	1
1:A:130:SER:C	1:A:131:CYS:O	0.43	2.62	14	5
1:A:75:THR:HG23	1:A:77:GLN:CD	0.43	2.39	21	1
1:A:53:ASP:OD1	1:A:54:GLN:NE2	0.43	2.52	2	1
1:A:29:TYR:HB2	1:A:149:LEU:CD2	0.43	2.44	9	2
1:A:55:HIS:NE2	1:A:74:GLU:OE2	0.43	2.51	12	1
1:A:124:GLY:C	1:A:125:LEU:HD23	0.43	2.39	16	1
1:A:138:HIS:ND1	1:A:138:HIS:N	0.43	2.66	1	1
1:A:147:LEU:HD22	1:A:148:PRO:HD2	0.43	1.91	3	1
1:A:53:ASP:O	1:A:54:GLN:C	0.43	2.62	8	2
1:A:74:GLU:OE1	1:A:74:GLU:CA	0.43	2.67	11	1
1:A:68:VAL:HG21	1:A:111:TYR:CE1	0.43	2.49	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:HIS:CE1	1:A:74:GLU:CG	0.43	3.02	23	1
1:A:27:LEU:CD1	1:A:36:PHE:CE1	0.43	3.02	26	1
1:A:36:PHE:CG	1:A:51:ARG:HD3	0.43	2.49	26	1
1:A:45:VAL:HG23	1:A:87:LEU:O	0.42	2.14	2	1
1:A:123:VAL:O	1:A:123:VAL:CG1	0.42	2.67	9	1
1:A:124:GLY:C	1:A:125:LEU:CD1	0.42	2.90	11	1
1:A:105:GLU:OE1	1:A:106:ASN:N	0.42	2.50	13	1
1:A:139:TYR:CD1	1:A:144:ILE:HD11	0.42	2.49	13	2
1:A:65:VAL:C	1:A:67:GLU:N	0.42	2.77	22	1
1:A:26:LYS:CD	1:A:59:GLN:OE1	0.42	2.66	24	1
1:A:68:VAL:CG2	1:A:101:GLU:HB2	0.42	2.43	12	2
1:A:137:THR:O	1:A:137:THR:OG1	0.42	2.34	10	4
1:A:39:ILE:O	1:A:40:LEU:HD13	0.42	2.14	2	2
1:A:62:ALA:CB	1:A:68:VAL:CG1	0.42	2.94	19	3
1:A:101:GLU:OE2	1:A:109:ASN:CB	0.42	2.67	5	1
1:A:138:HIS:O	2:A:178:NTS:O62	0.42	2.37	16	5
1:A:54:GLN:NE2	1:A:55:HIS:O	0.42	2.51	6	1
1:A:124:GLY:HA2	1:A:146:PHE:CZ	0.42	2.49	26	2
1:A:85:GLY:HA3	1:A:121:TRP:CZ3	0.42	2.49	13	1
1:A:38:ARG:NH2	1:A:53:ASP:OD2	0.42	2.52	15	1
1:A:139:TYR:O	2:A:178:NTS:O63	0.42	2.37	20	2
1:A:78:TYR:CE2	1:A:93:PRO:HG3	0.42	2.49	22	1
1:A:26:LYS:CG	1:A:150:PRO:HB3	0.42	2.43	24	3
1:A:113:SER:C	1:A:115:LYS:N	0.42	2.77	8	2
1:A:139:TYR:HA	2:A:178:NTS:O62	0.42	2.14	19	1
1:A:107:HIS:O	1:A:108:TYR:C	0.42	2.61	23	1
1:A:87:LEU:N	1:A:87:LEU:CD1	0.42	2.82	3	1
1:A:101:GLU:C	1:A:102:ARG:CG	0.42	2.92	20	2
1:A:139:TYR:O	2:A:178:NTS:O62	0.42	2.38	16	2
1:A:39:ILE:HD11	1:A:79:LEU:HD22	0.42	1.90	7	1
1:A:102:ARG:NH2	1:A:122:PHE:CZ	0.42	2.87	9	1
1:A:38:ARG:NH2	1:A:53:ASP:OD1	0.42	2.52	24	2
1:A:145:LEU:HD21	2:A:178:NTS:O61	0.42	2.14	13	1
1:A:26:LYS:HG3	1:A:150:PRO:CA	0.42	2.45	6	2
1:A:35:HIS:HB3	1:A:48:THR:C	0.42	2.39	19	2
1:A:145:LEU:CD2	2:A:178:NTS:O61	0.42	2.67	13	1
1:A:39:ILE:CD1	1:A:79:LEU:HD12	0.42	2.44	14	1
1:A:70:ILE:CG2	1:A:79:LEU:HB3	0.42	2.44	17	1
1:A:39:ILE:HD13	1:A:72:SER:HB3	0.42	1.91	3	1
1:A:39:ILE:HG23	1:A:77:GLN:OE1	0.42	2.14	12	1
1:A:101:GLU:OE2	1:A:102:ARG:O	0.42	2.38	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:TYR:C	1:A:109:ASN:CG	0.42	2.88	1	1
1:A:111:TYR:HB2	1:A:123:VAL:CG1	0.42	2.44	17	6
1:A:66:GLY:O	1:A:67:GLU:OE1	0.42	2.38	4	2
1:A:45:VAL:HG11	1:A:87:LEU:C	0.42	2.40	6	2
1:A:71:LYS:HG2	1:A:78:TYR:CG	0.42	2.50	8	2
1:A:112:ILE:HG22	1:A:117:ALA:CB	0.42	2.45	12	2
1:A:58:LEU:O	1:A:73:THR:OG1	0.42	2.38	25	2
1:A:107:HIS:O	1:A:108:TYR:O	0.42	2.38	22	5
1:A:27:LEU:O	1:A:27:LEU:HG	0.42	2.14	6	2
1:A:38:ARG:HA	1:A:56:ILE:HA	0.42	1.92	10	2
1:A:38:ARG:N	1:A:46:ASP:O	0.42	2.48	12	1
1:A:68:VAL:CG1	1:A:101:GLU:OE1	0.42	2.63	15	1
1:A:127:LYS:C	1:A:127:LYS:HD3	0.42	2.39	6	2
1:A:113:SER:HB2	1:A:116:HIS:CE1	0.42	2.50	10	1
1:A:93:PRO:HA	1:A:97:CYS:SG	0.42	2.55	13	2
1:A:147:LEU:CD2	1:A:148:PRO:HD2	0.42	2.45	13	1
1:A:132:LYS:CG	1:A:136:ARG:HB3	0.42	2.45	18	1
1:A:26:LYS:HE3	1:A:27:LEU:N	0.42	2.30	20	1
1:A:71:LYS:C	1:A:71:LYS:HE3	0.42	2.39	25	1
1:A:46:ASP:O	1:A:125:LEU:CD2	0.42	2.68	3	1
1:A:74:GLU:CD	1:A:75:THR:HG23	0.42	2.40	4	1
1:A:124:GLY:C	1:A:125:LEU:CG	0.42	2.93	5	1
1:A:124:GLY:HA3	1:A:144:ILE:HG22	0.42	1.92	5	1
1:A:62:ALA:HB1	1:A:68:VAL:HG12	0.42	1.91	19	2
1:A:78:TYR:CB	1:A:97:CYS:SG	0.42	3.08	15	1
1:A:27:LEU:HD11	1:A:36:PHE:CE2	0.42	2.49	18	1
1:A:69:TYR:CE1	1:A:98:LEU:CD1	0.42	3.03	19	1
1:A:131:CYS:O	1:A:132:LYS:CD	0.42	2.67	21	1
1:A:150:PRO:C	1:A:151:VAL:HG13	0.41	2.39	11	2
1:A:55:HIS:ND1	1:A:57:GLN:OE1	0.41	2.50	12	1
1:A:125:LEU:HD13	1:A:131:CYS:HA	0.41	1.91	16	1
1:A:57:GLN:C	1:A:58:LEU:HG	0.41	2.40	17	1
1:A:67:GLU:CG	1:A:114:LYS:CE	0.41	2.98	24	1
1:A:81:MET:O	1:A:116:HIS:NE2	0.41	2.53	25	1
1:A:132:LYS:HB2	1:A:137:THR:HG23	0.41	1.92	5	1
1:A:145:LEU:HD23	1:A:145:LEU:H	0.41	1.74	5	1
1:A:45:VAL:CG1	1:A:87:LEU:C	0.41	2.93	19	3
1:A:29:TYR:CG	1:A:36:PHE:CE2	0.41	3.08	7	1
1:A:31:SER:CB	1:A:145:LEU:HB3	0.41	2.45	12	1
1:A:83:THR:CG2	1:A:115:LYS:NZ	0.41	2.83	13	1
1:A:44:THR:HG22	1:A:45:VAL:N	0.41	2.30	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:SER:O	1:A:116:HIS:N	0.41	2.46	8	1
1:A:59:GLN:O	1:A:71:LYS:N	0.41	2.50	17	1
1:A:70:ILE:CG2	1:A:79:LEU:HB2	0.41	2.45	3	6
1:A:26:LYS:HZ1	1:A:28:LEU:HD12	0.41	1.76	7	1
1:A:39:ILE:CD1	1:A:79:LEU:HD22	0.41	2.45	12	1
1:A:38:ARG:CZ	1:A:53:ASP:OD2	0.41	2.68	21	1
1:A:60:LEU:CD2	1:A:70:ILE:HG12	0.41	2.45	21	1
1:A:68:VAL:CG2	1:A:101:GLU:CB	0.41	2.99	1	1
1:A:67:GLU:HG3	1:A:114:LYS:CD	0.41	2.46	2	1
1:A:137:THR:OG1	1:A:137:THR:O	0.41	2.38	3	2
1:A:138:HIS:O	2:A:178:NTS:O61	0.41	2.39	4	1
1:A:81:MET:HE2	1:A:121:TRP:HB3	0.41	1.92	5	1
1:A:46:ASP:HA	1:A:125:LEU:CD2	0.41	2.45	19	1
1:A:132:LYS:CD	1:A:136:ARG:O	0.41	2.69	20	1
1:A:41:PRO:CD	1:A:55:HIS:NE2	0.41	2.84	4	1
1:A:53:ASP:OD2	1:A:54:GLN:OE1	0.41	2.38	6	1
1:A:55:HIS:CG	1:A:74:GLU:CG	0.41	3.04	12	1
1:A:121:TRP:CZ2	1:A:135:PRO:HB3	0.41	2.50	17	1
1:A:30:CYS:SG	1:A:35:HIS:O	0.41	2.78	14	1
1:A:144:ILE:HD11	2:A:178:NTS:O62	0.41	2.16	15	1
1:A:145:LEU:HD12	1:A:145:LEU:HA	0.41	1.82	24	1
1:A:38:ARG:CD	1:A:48:THR:OG1	0.41	2.68	26	1
1:A:100:LEU:HB3	1:A:112:ILE:HG22	0.41	1.93	9	1
1:A:122:PHE:CE2	1:A:144:ILE:CD1	0.41	3.04	12	1
1:A:123:VAL:CG2	1:A:123:VAL:O	0.41	2.68	14	1
1:A:70:ILE:CG2	1:A:79:LEU:CB	0.41	2.98	24	1
1:A:62:ALA:HA	1:A:68:VAL:CB	0.41	2.46	1	2
1:A:124:GLY:O	1:A:131:CYS:SG	0.41	2.79	1	1
1:A:59:GLN:OE1	1:A:73:THR:HG21	0.41	2.16	2	1
1:A:127:LYS:HD2	1:A:127:LYS:C	0.41	2.41	3	2
1:A:54:GLN:HG2	1:A:55:HIS:CD2	0.41	2.51	4	1
1:A:139:TYR:O	2:A:178:NTS:O61	0.41	2.38	4	1
1:A:67:GLU:OE1	1:A:114:LYS:NZ	0.41	2.52	5	1
1:A:105:GLU:HG2	1:A:107:HIS:CE1	0.41	2.50	23	2
1:A:130:SER:O	1:A:131:CYS:O	0.41	2.39	22	4
1:A:38:ARG:HB3	1:A:56:ILE:CG2	0.41	2.46	7	1
1:A:51:ARG:O	1:A:51:ARG:CZ	0.41	2.69	7	1
1:A:124:GLY:HA3	1:A:144:ILE:N	0.41	2.31	21	3
1:A:29:TYR:O	1:A:147:LEU:N	0.41	2.50	13	1
1:A:139:TYR:CD1	2:A:178:NTS:O63	0.41	2.74	13	1
1:A:73:THR:O	1:A:74:GLU:HB2	0.41	2.16	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLU:OE2	1:A:105:GLU:N	0.41	2.54	16	1
1:A:35:HIS:N	1:A:35:HIS:ND1	0.41	2.69	18	1
1:A:75:THR:O	1:A:76:GLY:O	0.41	2.38	18	2
1:A:57:GLN:OE1	1:A:73:THR:O	0.41	2.39	20	1
1:A:29:TYR:CG	1:A:30:CYS:N	0.41	2.89	21	1
1:A:104:GLU:HG2	1:A:145:LEU:HD21	0.41	1.92	21	1
1:A:110:THR:CG2	1:A:145:LEU:CD2	0.41	2.99	22	1
1:A:35:HIS:ND1	1:A:35:HIS:N	0.41	2.69	26	1
1:A:27:LEU:CD1	1:A:149:LEU:HD11	0.41	2.44	1	1
1:A:67:GLU:CD	1:A:114:LYS:HE3	0.41	2.41	3	2
1:A:150:PRO:C	1:A:151:VAL:CG2	0.41	2.94	14	1
1:A:104:GLU:OE2	1:A:105:GLU:CA	0.41	2.69	16	1
1:A:97:CYS:C	1:A:98:LEU:O	0.41	2.64	23	1
1:A:138:HIS:O	2:A:178:NTS:C7	0.41	2.69	24	1
1:A:67:GLU:CG	1:A:114:LYS:HD2	0.40	2.45	2	1
1:A:81:MET:C	1:A:82:ASP:O	0.40	2.64	3	1
1:A:29:TYR:CE2	1:A:31:SER:O	0.40	2.73	7	1
1:A:56:ILE:HD13	1:A:56:ILE:C	0.40	2.42	8	1
1:A:30:CYS:SG	1:A:125:LEU:CD1	0.40	3.09	11	1
1:A:26:LYS:HE3	1:A:27:LEU:CA	0.40	2.46	12	1
1:A:85:GLY:N	1:A:121:TRP:CZ3	0.40	2.90	13	1
1:A:67:GLU:HG3	1:A:114:LYS:CE	0.40	2.46	16	1
1:A:111:TYR:C	1:A:112:ILE:CG1	0.40	2.94	23	1
1:A:68:VAL:CG2	1:A:111:TYR:CE2	0.40	2.95	26	1
1:A:86:LEU:HD12	1:A:133:ARG:HB2	0.40	1.93	1	1
1:A:27:LEU:CD2	1:A:51:ARG:NH2	0.40	2.84	2	1
1:A:78:TYR:O	1:A:89:GLY:HA2	0.40	2.17	12	1
1:A:68:VAL:N	1:A:98:LEU:HD23	0.40	2.31	15	1
1:A:71:LYS:CG	1:A:78:TYR:CZ	0.40	3.05	15	1
1:A:100:LEU:HD12	1:A:114:LYS:HG3	0.40	1.94	18	1
1:A:104:GLU:C	1:A:104:GLU:OE1	0.40	2.64	21	1
1:A:83:THR:HG23	1:A:115:LYS:HZ3	0.40	1.73	24	1
1:A:127:LYS:C	1:A:127:LYS:CD	0.40	2.94	3	1
1:A:69:TYR:CE1	1:A:98:LEU:HD22	0.40	2.52	4	1
1:A:37:LEU:HB3	1:A:58:LEU:CD1	0.40	2.45	6	1
1:A:73:THR:O	1:A:74:GLU:OE1	0.40	2.39	8	2
1:A:83:THR:HA	1:A:116:HIS:NE2	0.40	2.31	15	1
1:A:39:ILE:HB	1:A:58:LEU:HD21	0.40	1.94	16	1
1:A:104:GLU:HB2	1:A:110:THR:OG1	0.40	2.16	18	1
1:A:110:THR:HG22	1:A:145:LEU:HA	0.40	1.93	18	1
1:A:108:TYR:CD1	1:A:108:TYR:N	0.40	2.86	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:TRP:NE1	1:A:135:PRO:HA	0.40	2.32	1	1
1:A:55:HIS:CE1	1:A:57:GLN:NE2	0.40	2.89	2	1
1:A:92:THR:O	1:A:92:THR:OG1	0.40	2.39	2	3
1:A:38:ARG:NH1	1:A:46:ASP:OD1	0.40	2.54	5	1
1:A:99:PHE:CD1	1:A:111:TYR:HB3	0.40	2.51	5	1
1:A:124:GLY:C	1:A:125:LEU:HG	0.40	2.40	5	1
1:A:132:LYS:HG2	1:A:136:ARG:CB	0.40	2.46	18	1
1:A:110:THR:HG22	1:A:144:ILE:HG13	0.40	1.92	21	1
1:A:88:TYR:OH	1:A:96:GLU:OE2	0.40	2.40	9	1
1:A:78:TYR:O	1:A:97:CYS:SG	0.40	2.80	20	1
1:A:54:GLN:CD	1:A:54:GLN:C	0.40	2.89	22	1
1:A:112:ILE:O	1:A:112:ILE:CG2	0.40	2.67	24	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/155 (77%)	72±3 (60±3%)	26±3 (22±2%)	21±2 (18±2%)	0	3
All	All	3094/4030 (77%)	1864 (60%)	682 (22%)	548 (18%)	0	3

All 46 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	74	GLU	26
1	A	107	HIS	26
1	A	151	VAL	26
1	A	113	SER	24
1	A	130	SER	23
1	A	31	SER	22
1	A	64	SER	22
1	A	139	TYR	22
1	A	136	ARG	21
1	A	103	LEU	21

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Mol	Chain	Res	Type	Models (Total)
1	A	73	THR	20
1	A	52	SER	19
1	A	127	LYS	19
1	A	37	LEU	18
1	A	100	LEU	17
1	A	129	GLY	16
1	A	116	HIS	14
1	A	46	ASP	13
1	A	96	GLU	13
1	A	98	LEU	13
1	A	108	TYR	12
1	A	121	TRP	12
1	A	126	LYS	12
1	A	102	ARG	12
1	A	72	SER	11
1	A	145	LEU	10
1	A	110	THR	10
1	A	131	CYS	10
1	A	76	GLY	9
1	A	43	GLY	8
1	A	51	ARG	8
1	A	122	PHE	7
1	A	82	ASP	7
1	A	95	GLU	5
1	A	55	HIS	4
1	A	26	LYS	2
1	A	75	THR	2
1	A	79	LEU	2
1	A	106	ASN	2
1	A	65	VAL	2
1	A	49	ARG	1
1	A	109	ASN	1
1	A	112	ILE	1
1	A	85	GLY	1
1	A	128	ASN	1
1	A	134	GLY	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/135 (79%)	61±3 (57±3%)	46±3 (43±3%)	0	4
All	All	2782/3510 (79%)	1592 (57%)	1190 (43%)	0	4

All 84 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	39	ILE	26
1	A	40	LEU	26
1	A	46	ASP	26
1	A	99	PHE	26
1	A	100	LEU	26
1	A	115	LYS	26
1	A	56	ILE	25
1	A	64	SER	25
1	A	71	LYS	25
1	A	77	GLN	25
1	A	28	LEU	24
1	A	63	GLU	24
1	A	147	LEU	24
1	A	125	LEU	24
1	A	37	LEU	23
1	A	45	VAL	23
1	A	60	LEU	23
1	A	81	MET	23
1	A	112	ILE	23
1	A	116	HIS	23
1	A	51	ARG	23
1	A	65	VAL	21
1	A	90	SER	21
1	A	127	LYS	21
1	A	27	LEU	20
1	A	102	ARG	20
1	A	26	LYS	20
1	A	119	LYS	20
1	A	120	ASN	20
1	A	136	ARG	19
1	A	151	VAL	19
1	A	44	THR	18
1	A	103	LEU	17
1	A	105	GLU	17
1	A	132	LYS	17
1	A	114	LYS	16

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Mol	Chain	Res	Type	Models (Total)
1	A	98	LEU	16
1	A	149	LEU	15
1	A	139	TYR	15
1	A	30	CYS	14
1	A	49	ARG	14
1	A	94	ASN	14
1	A	54	GLN	13
1	A	133	ARG	13
1	A	137	THR	13
1	A	138	HIS	13
1	A	95	GLU	13
1	A	91	GLN	12
1	A	101	GLU	12
1	A	57	GLN	11
1	A	55	HIS	11
1	A	131	CYS	11
1	A	50	ASP	10
1	A	74	GLU	10
1	A	42	ASP	9
1	A	73	THR	9
1	A	128	ASN	9
1	A	38	ARG	8
1	A	84	ASP	8
1	A	59	GLN	8
1	A	48	THR	7
1	A	145	LEU	7
1	A	79	LEU	7
1	A	104	GLU	7
1	A	126	LYS	7
1	A	58	LEU	7
1	A	75	THR	6
1	A	86	LEU	6
1	A	88	TYR	6
1	A	53	ASP	6
1	A	67	GLU	6
1	A	144	ILE	6
1	A	31	SER	5
1	A	130	SER	5
1	A	87	LEU	4
1	A	97	CYS	4
1	A	107	HIS	3
1	A	111	TYR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	52	SER	2
1	A	83	THR	2
1	A	108	TYR	1
1	A	35	HIS	1
1	A	61	SER	1
1	A	110	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	NTS	A	178	-	22,23,23	4.84±0.00	11±0 (50±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of

the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NTS	A	178	-	36,38,38	0.82±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NTS	A	178	-	-	0±0,18,18,18	0±0,2,2,2

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	178	NTS	O61-S6	7.68	1.80	1.43	26	26
2	A	178	NTS	O31-S3	7.67	1.80	1.43	22	26
2	A	178	NTS	O32-S3	7.67	1.80	1.43	16	26
2	A	178	NTS	O12-S1	7.67	1.80	1.43	12	26
2	A	178	NTS	O11-S1	7.66	1.80	1.43	4	26
2	A	178	NTS	O62-S6	7.65	1.80	1.43	5	26
2	A	178	NTS	O13-S1	6.71	1.80	1.45	23	26
2	A	178	NTS	O33-S3	6.71	1.80	1.45	10	26
2	A	178	NTS	O63-S6	6.70	1.80	1.45	10	26
2	A	178	NTS	C6-S6	2.58	1.82	1.77	25	26
2	A	178	NTS	C3-S3	2.58	1.82	1.77	24	26

There are no bond-angle outliers.

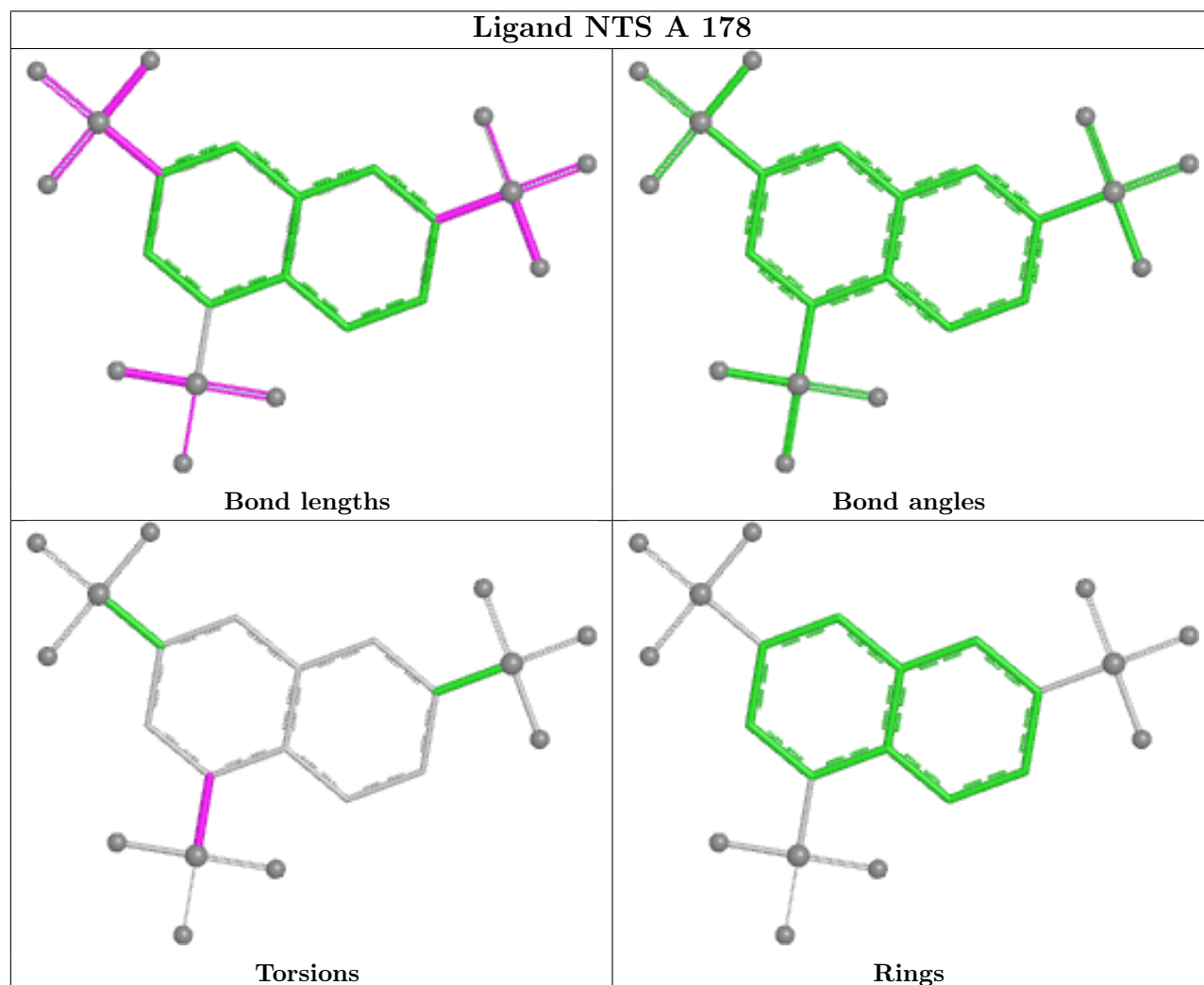
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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