



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 02:06 AM UTC

PDB ID : 2KT4 / pdb_00002kt4
Title : Lipocalin Q83 is a Siderocalin
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Deposited on : 2010-01-18

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<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

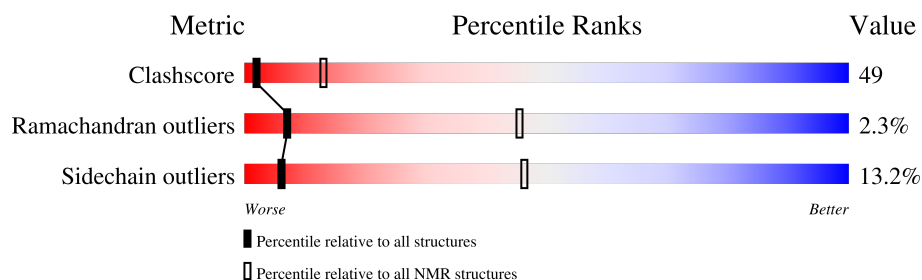
1 Overall quality at a glance

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	B	157	

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:1-B:157 (157)	0.41	14

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

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

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

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2596 atoms, of which 1281 are hydrogens and 0 are deuteriums.

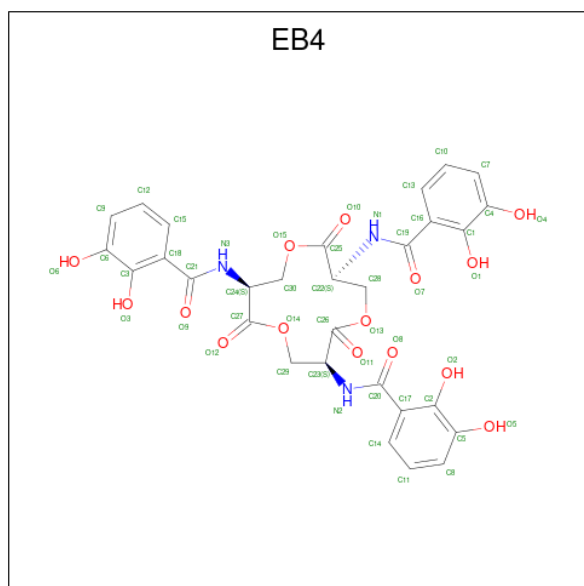
- Molecule 1 is a protein called Extracellular fatty acid-binding protein.

Mol	Chain	Residues	Atoms						Trace
1	B	157	Total	C	H	N	O	S	0
			2526	799	1260	213	244	10	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9I9P7

- Molecule 2 is N,N',N''-[(3S,7S,11S)-2,6,10-trioxo-1,5,9-trioxacyclododecane-3,7,11-triyl]tris(2,3-dihydroxybenzamide) (CCD ID: EB4) (formula: C₃₀H₂₇N₃O₁₅).



Mol	Chain	Residues	Atoms				
2	B	1	Total	C	H	N	O
			69	30	21	3	15

- Molecule 3 is GALLIUM (III) ION (CCD ID: GA) (formula: Ga).

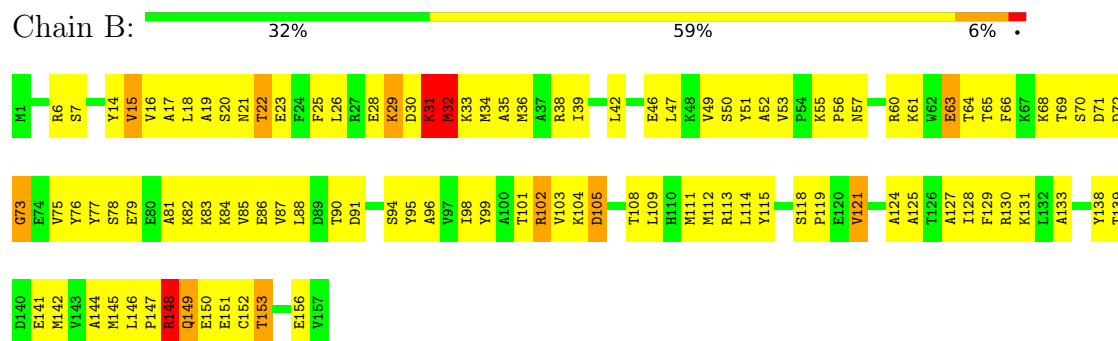
Mol	Chain	Residues	Atoms	
3	B	1	Total	Ga
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Extracellular fatty acid-binding protein

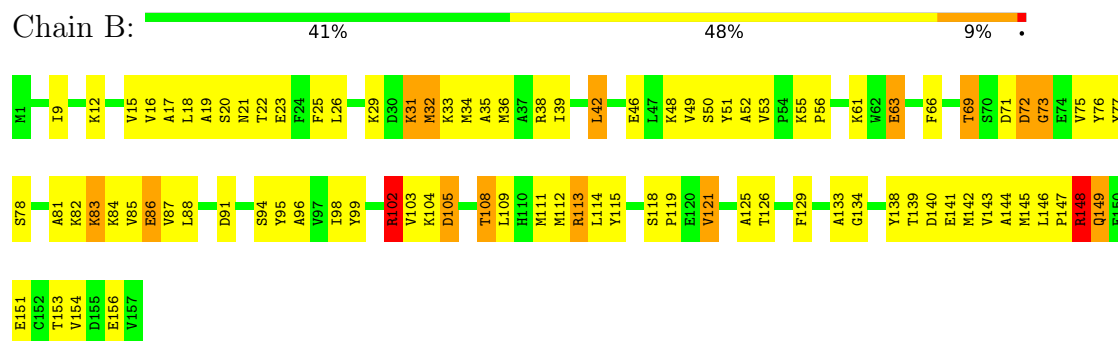


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

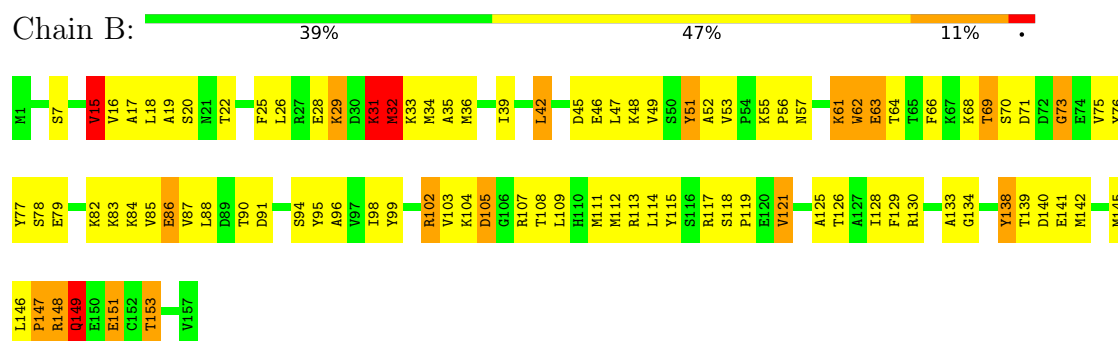
4.2.1 Score per residue for model 1

- Molecule 1: Extracellular fatty acid-binding protein



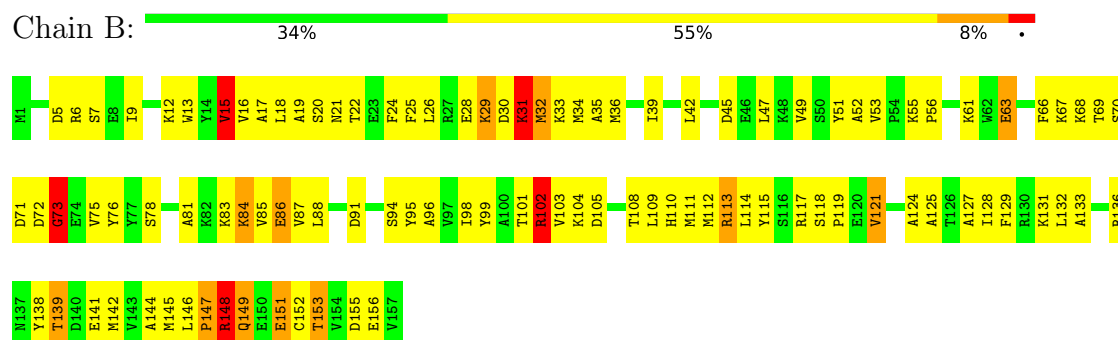
4.2.2 Score per residue for model 2

- Molecule 1: Extracellular fatty acid-binding protein



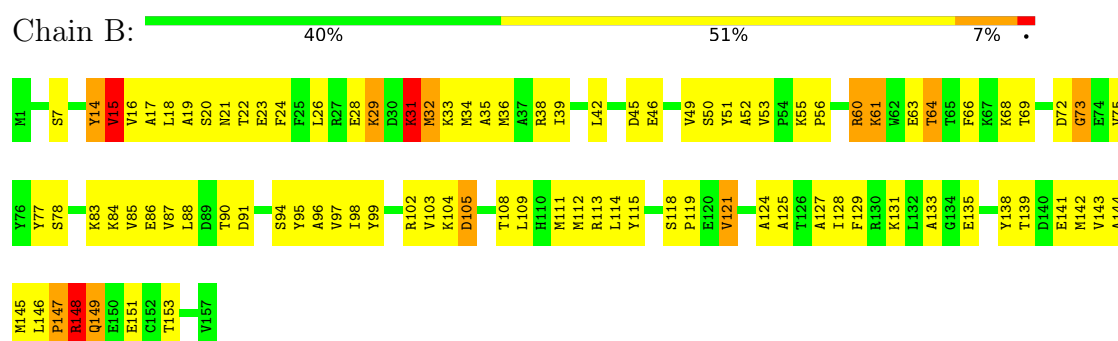
4.2.3 Score per residue for model 3

- Molecule 1: Extracellular fatty acid-binding protein



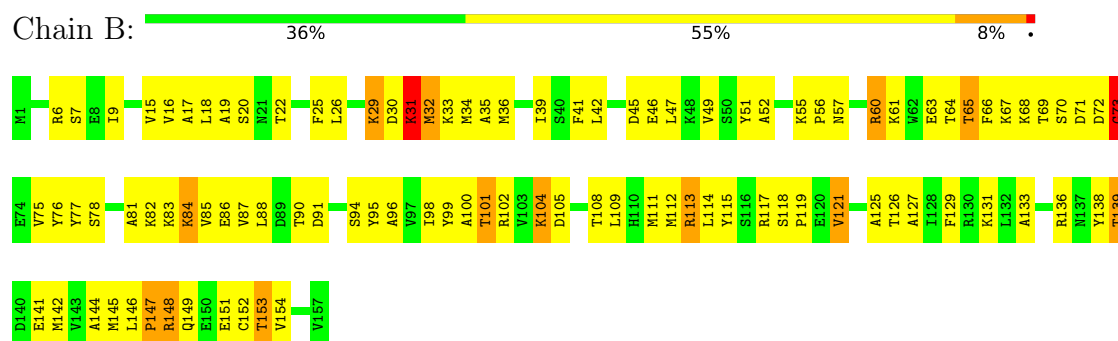
4.2.4 Score per residue for model 4

- Molecule 1: Extracellular fatty acid-binding protein



4.2.5 Score per residue for model 5

- Molecule 1: Extracellular fatty acid-binding protein



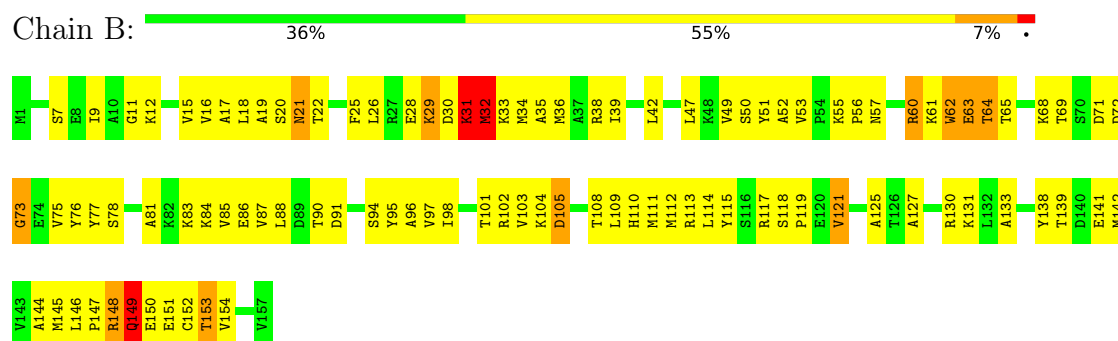
4.2.6 Score per residue for model 6

- Molecule 1: Extracellular fatty acid-binding protein



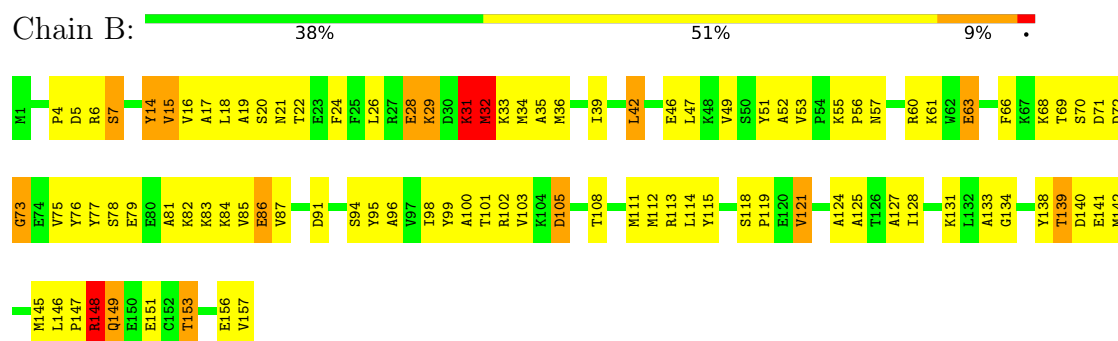
4.2.7 Score per residue for model 7

- Molecule 1: Extracellular fatty acid-binding protein



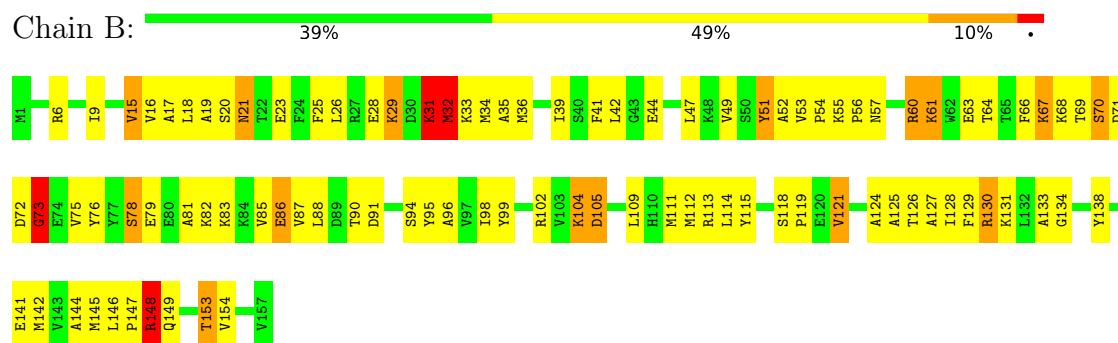
4.2.8 Score per residue for model 8

- Molecule 1: Extracellular fatty acid-binding protein



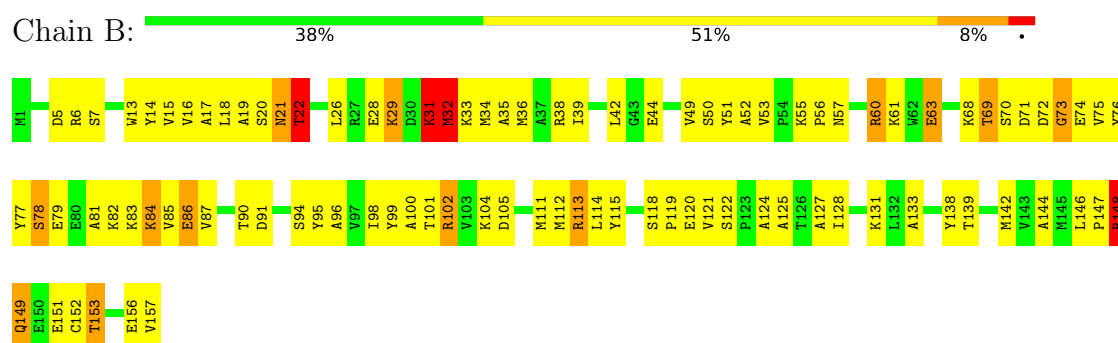
4.2.9 Score per residue for model 9

- Molecule 1: Extracellular fatty acid-binding protein



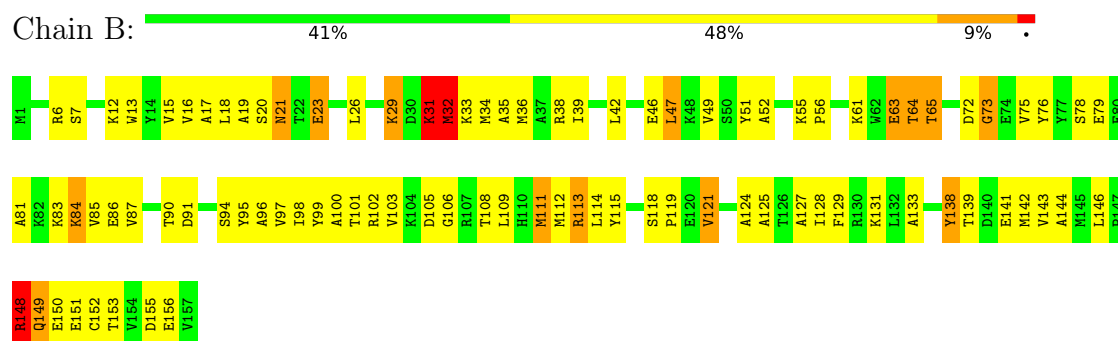
4.2.10 Score per residue for model 10

- Molecule 1: Extracellular fatty acid-binding protein



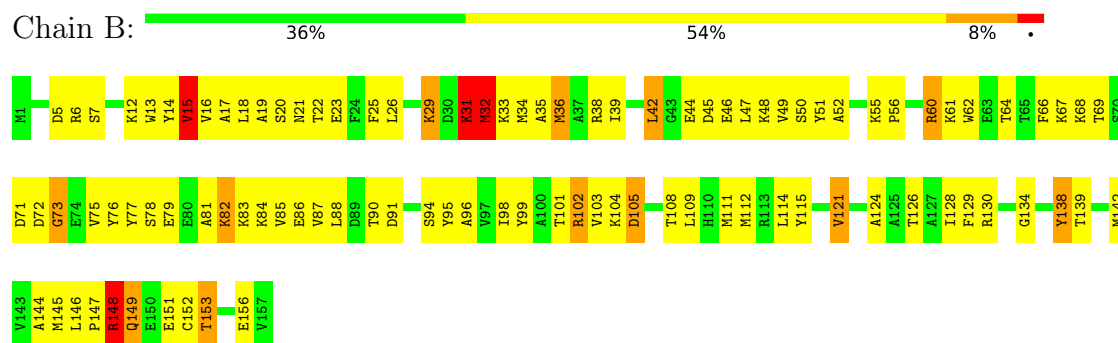
4.2.11 Score per residue for model 11

- Molecule 1: Extracellular fatty acid-binding protein



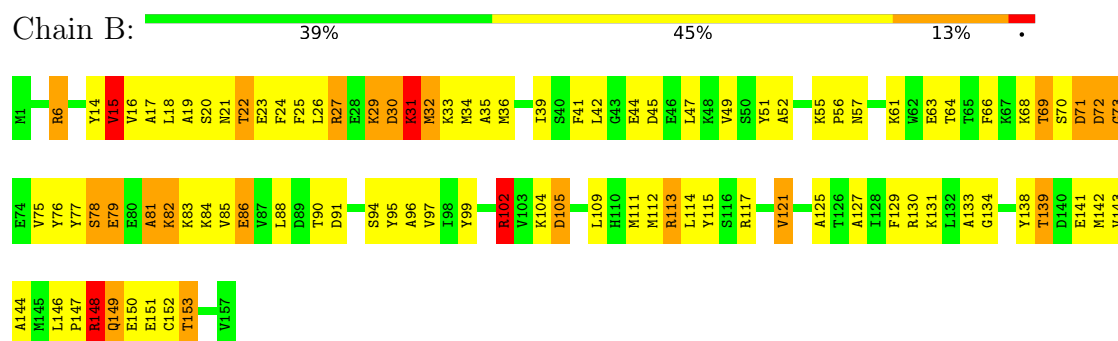
4.2.12 Score per residue for model 12

- Molecule 1: Extracellular fatty acid-binding protein



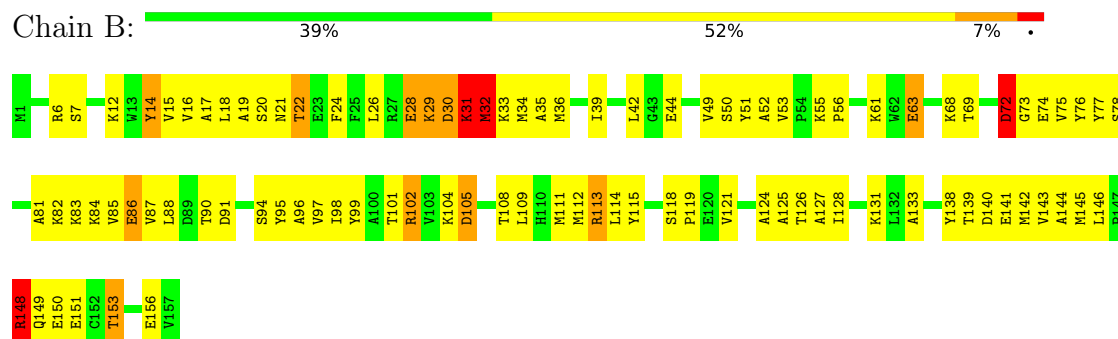
4.2.13 Score per residue for model 13

- Molecule 1: Extracellular fatty acid-binding protein



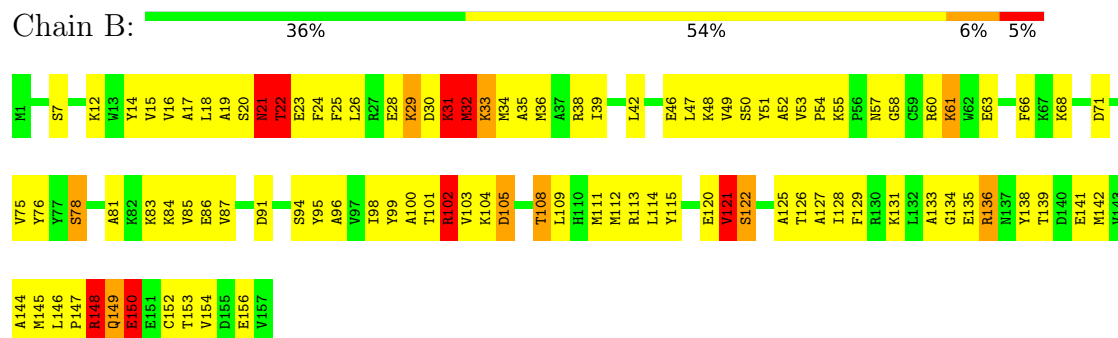
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Extracellular fatty acid-binding protein



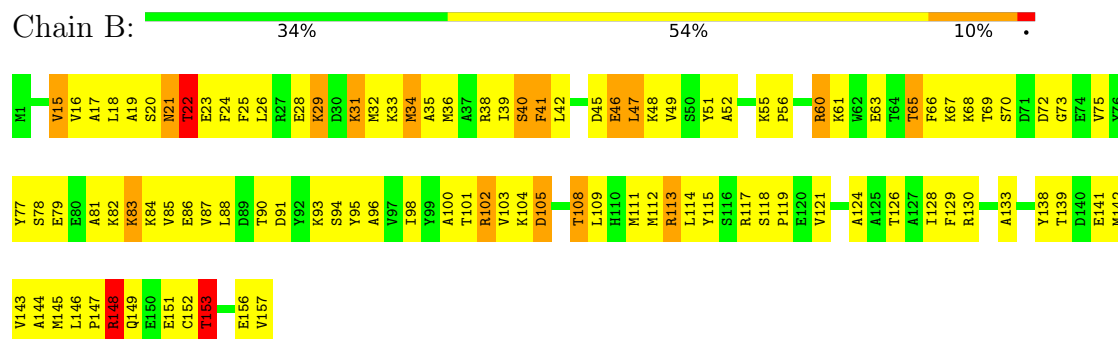
4.2.15 Score per residue for model 15

- Molecule 1: Extracellular fatty acid-binding protein



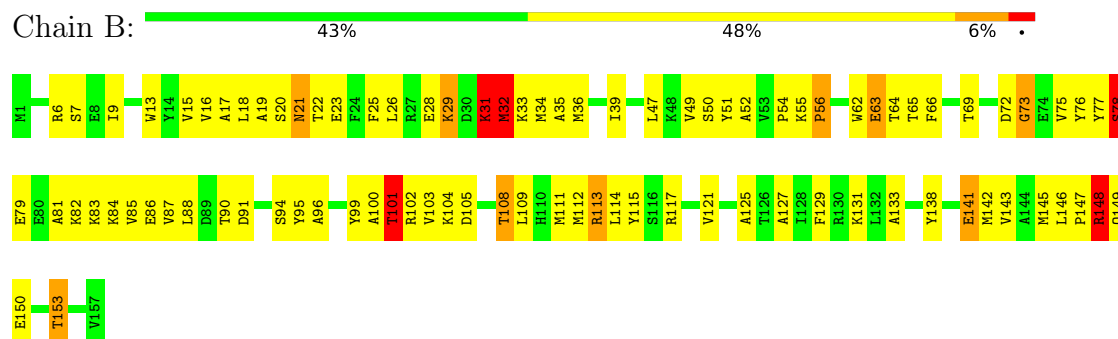
4.2.16 Score per residue for model 16

- Molecule 1: Extracellular fatty acid-binding protein



4.2.17 Score per residue for model 17

- Molecule 1: Extracellular fatty acid-binding protein



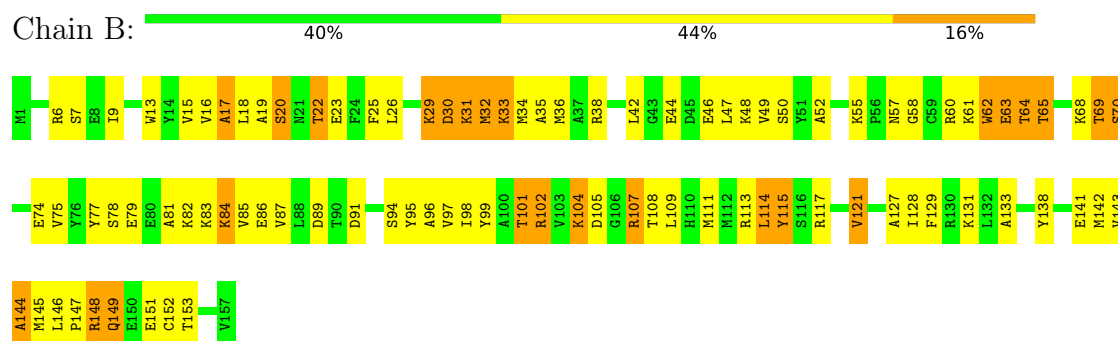
4.2.18 Score per residue for model 18

- Molecule 1: Extracellular fatty acid-binding protein



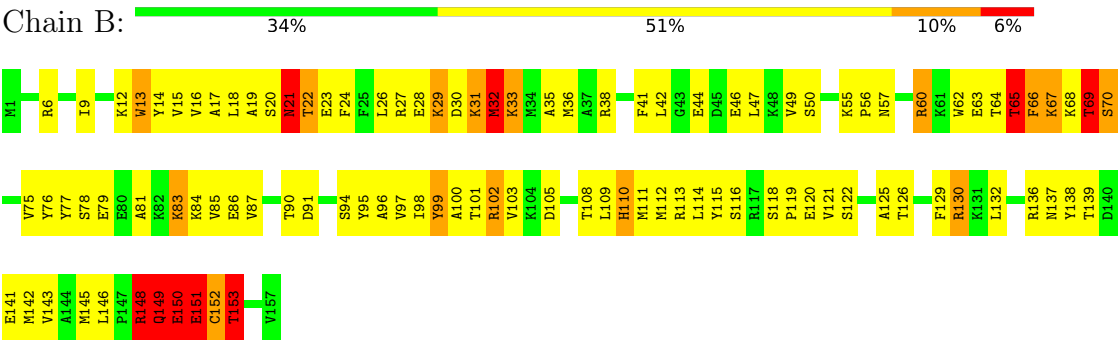
4.2.19 Score per residue for model 19

- Molecule 1: Extracellular fatty acid-binding protein



4.2.20 Score per residue for model 20

- Molecule 1: Extracellular fatty acid-binding protein



5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

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

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: EB4, GA

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	B	0.67±0.08	2±2/1290 (0.2± 0.1%)	1.00±0.11	9±3/1735 (0.5± 0.2%)
All	All	0.68	42/25800 (0.2%)	1.01	179/34700 (0.5%)

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	B	0.1±0.3	5.3±2.2
All	All	2	107

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
1	B	73	GLY	C-N	9.60	1.46	1.33	14	1
1	B	72	ASP	C-O	-9.22	1.11	1.24	14	2
1	B	73	GLY	N-CA	-7.72	1.37	1.45	14	1
1	B	31	LYS	C-N	7.18	1.43	1.33	8	5
1	B	32	MET	CA-CB	7.14	1.65	1.53	11	10
1	B	122	SER	CA-C	6.74	1.60	1.52	18	2
1	B	121	VAL	CA-C	-6.67	1.44	1.52	18	1
1	B	121	VAL	CA-CB	6.39	1.62	1.54	18	1
1	B	72	ASP	N-CA	6.06	1.54	1.46	14	1
1	B	150	GLU	N-CA	-6.01	1.38	1.46	15	2
1	B	15	VAL	CA-CB	5.97	1.60	1.53	13	6
1	B	152	CYS	N-CA	-5.79	1.39	1.46	20	1
1	B	72	ASP	C-N	-5.60	1.25	1.33	12	2
1	B	73	GLY	C-O	-5.47	1.17	1.24	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	121	VAL	C-O	5.36	1.31	1.24	18	1
1	B	148	ARG	N-CA	5.23	1.52	1.46	17	1
1	B	32	MET	CA-C	5.21	1.59	1.52	6	1
1	B	148	ARG	CA-C	5.18	1.59	1.52	20	1
1	B	22	THR	N-CA	5.12	1.52	1.46	18	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	B	73	GLY	O-C-N	-18.07	108.25	122.71	14	3
1	B	73	GLY	CA-C-O	-12.33	109.35	119.83	14	15
1	B	74	GLU	N-CA-CB	10.71	122.66	110.35	14	1
1	B	149	GLN	CA-C-N	-10.65	108.61	122.77	15	3
1	B	149	GLN	C-N-CA	-10.65	108.61	122.77	15	3
1	B	73	GLY	CA-C-N	-10.59	106.78	122.24	14	2
1	B	73	GLY	C-N-CA	-10.59	106.78	122.24	14	2
1	B	31	LYS	CA-C-N	-8.94	104.47	121.54	17	16
1	B	31	LYS	C-N-CA	-8.94	104.47	121.54	17	16
1	B	152	CYS	CA-C-N	8.42	139.42	123.09	16	1
1	B	152	CYS	C-N-CA	8.42	139.42	123.09	16	1
1	B	72	ASP	CA-C-N	8.38	137.84	121.41	12	14
1	B	72	ASP	C-N-CA	8.38	137.84	121.41	12	14
1	B	150	GLU	N-CA-C	8.36	121.99	109.95	20	1
1	B	32	MET	N-CA-CB	-8.36	96.36	110.49	14	16
1	B	22	THR	CA-C-O	-8.31	111.10	120.32	10	1
1	B	153	THR	N-CA-CB	7.98	124.06	110.65	16	1
1	B	148	ARG	CA-C-N	7.70	138.18	122.55	20	1
1	B	148	ARG	C-N-CA	7.70	138.18	122.55	20	1
1	B	22	THR	N-CA-C	7.20	121.56	109.76	15	4
1	B	149	GLN	N-CA-C	7.15	121.43	113.21	20	2
1	B	152	CYS	O-C-N	6.95	132.03	123.21	16	1
1	B	121	VAL	N-CA-CB	6.77	119.90	110.56	18	2
1	B	72	ASP	O-C-N	6.38	130.58	121.97	16	1
1	B	32	MET	O-C-N	-6.12	114.45	122.59	14	3
1	B	150	GLU	N-CA-CB	-6.12	100.45	110.42	15	2
1	B	41	PHE	N-CA-C	6.10	118.79	107.99	16	1
1	B	108	THR	N-CA-C	5.93	118.19	108.52	18	1
1	B	14	TYR	CA-C-N	-5.82	115.09	122.37	4	6
1	B	14	TYR	C-N-CA	-5.82	115.09	122.37	4	6
1	B	111	MET	CA-C-N	-5.79	115.00	123.00	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	111	MET	C-N-CA	-5.79	115.00	123.00	18	1
1	B	149	GLN	N-CA-CB	5.75	118.90	110.57	20	1
1	B	22	THR	CB-CA-C	5.64	119.48	109.72	17	4
1	B	121	VAL	CB-CA-C	-5.63	103.35	111.34	8	13
1	B	109	LEU	N-CA-CB	5.54	118.84	110.42	18	1
1	B	151	GLU	CA-C-N	-5.52	115.43	122.77	20	1
1	B	151	GLU	C-N-CA	-5.52	115.43	122.77	20	1
1	B	41	PHE	CA-C-O	-5.47	114.61	120.46	16	1
1	B	74	GLU	N-CA-C	-5.46	103.76	110.65	14	1
1	B	122	SER	N-CA-C	5.46	118.28	109.15	15	1
1	B	66	PHE	CA-CB-CG	5.26	119.06	113.80	20	1
1	B	116	SER	N-CA-C	-5.24	101.62	109.95	20	1
1	B	32	MET	CA-C-O	-5.13	113.17	120.51	5	4
1	B	153	THR	CA-C-N	-5.12	114.59	122.68	16	1
1	B	153	THR	C-N-CA	-5.12	114.59	122.68	16	1
1	B	148	ARG	O-C-N	5.12	129.40	122.59	20	1
1	B	122	SER	CB-CA-C	5.08	115.99	110.15	15	1
1	B	149	GLN	CB-CA-C	5.05	119.66	110.72	20	1
1	B	101	THR	CB-CA-C	5.00	120.67	109.56	17	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	153	THR	CA	1
1	B	149	GLN	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	32	MET	Mainchain	16
1	B	73	GLY	Mainchain	14
1	B	149	GLN	Mainchain	12
1	B	102	ARG	Sidechain	7
1	B	15	VAL	Mainchain	7
1	B	21	ASN	Mainchain	6
1	B	151	GLU	Mainchain	5
1	B	150	GLU	Mainchain	4
1	B	62	TRP	Mainchain	3
1	B	69	THR	Mainchain	3
1	B	148	ARG	Mainchain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	121	VAL	Mainchain	2
1	B	153	THR	Mainchain	2
1	B	104	LYS	Mainchain	1
1	B	64	THR	Mainchain	1
1	B	22	THR	Mainchain	1
1	B	106	GLY	Mainchain	1
1	B	111	MET	Mainchain	1
1	B	24	PHE	Mainchain	1
1	B	71	ASP	Mainchain	1
1	B	81	ALA	Mainchain	1
1	B	72	ASP	Mainchain	1
1	B	33	LYS	Mainchain	1
1	B	34	MET	Mainchain	1
1	B	40	SER	Mainchain	1
1	B	46	GLU	Mainchain	1
1	B	47	LEU	Mainchain	1
1	B	78	SER	Mainchain	1
1	B	17	ALA	Mainchain	1
1	B	20	SER	Mainchain	1
1	B	114	LEU	Mainchain	1
1	B	144	ALA	Mainchain	1
1	B	65	THR	Mainchain	1
1	B	99	TYR	Mainchain	1
1	B	110	HIS	Mainchain	1
1	B	152	CYS	Mainchain	1

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	B	1266	1260	1261	126±15
2	B	48	21	21	12±4
All	All	26300	25620	25640	2532

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 49.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:84:LYS:HG3	1:B:101:THR:CB	1.17	1.68	17	2
1:B:102:ARG:HD3	2:B:158:EB4:C13	1.15	1.70	10	8
1:B:102:ARG:HD2	2:B:158:EB4:C13	1.13	1.74	3	8
1:B:102:ARG:HB2	1:B:109:LEU:HB3	1.11	1.16	17	1
1:B:102:ARG:CB	1:B:109:LEU:HB2	1.11	1.73	19	1
1:B:36:MET:HB2	1:B:52:ALA:HB3	1.10	1.15	7	18
1:B:103:VAL:HG22	1:B:108:THR:HG23	1.08	1.23	4	9
1:B:16:VAL:HB	1:B:121:VAL:HG22	1.08	1.22	3	17
1:B:26:LEU:HD22	1:B:142:MET:HA	1.08	1.21	19	7
1:B:102:ARG:HD2	2:B:158:EB4:H13	1.08	1.13	3	7
1:B:84:LYS:HG3	1:B:101:THR:HB	1.06	1.16	17	3
1:B:17:ALA:HB3	1:B:114:LEU:HB3	1.05	1.17	5	20
1:B:99:TYR:CD2	1:B:112:MET:HB2	1.05	1.85	18	1
1:B:34:MET:HG3	1:B:146:LEU:HB2	1.05	1.22	16	1
1:B:84:LYS:HE3	1:B:101:THR:HB	1.03	1.21	20	2
1:B:83:LYS:HG2	1:B:102:ARG:HG3	1.01	1.31	7	4
1:B:39:ILE:HG23	1:B:49:VAL:HG12	1.01	1.30	12	15
1:B:74:GLU:HB3	1:B:87:VAL:CG1	1.01	1.85	19	1
1:B:16:VAL:HB	1:B:121:VAL:CG2	1.00	1.87	19	17
1:B:18:LEU:HD13	1:B:29:LYS:HD3	0.99	1.30	9	15
1:B:102:ARG:HG2	1:B:109:LEU:HB3	0.98	1.35	13	7
1:B:16:VAL:CB	1:B:121:VAL:HG22	0.98	1.88	19	17
1:B:84:LYS:CG	1:B:101:THR:HB	0.97	1.87	17	5
1:B:81:ALA:CB	1:B:83:LYS:HE3	0.97	1.90	13	6
1:B:103:VAL:HG12	1:B:108:THR:HG23	0.96	1.35	3	1
1:B:31:LYS:HA	1:B:31:LYS:HE2	0.96	1.34	2	6
1:B:81:ALA:HB1	1:B:83:LYS:HE3	0.96	1.37	9	14
1:B:66:PHE:HD1	1:B:78:SER:HB3	0.95	1.21	4	2
1:B:85:VAL:HG12	1:B:100:ALA:CB	0.94	1.92	18	3
1:B:29:LYS:HE3	1:B:29:LYS:HA	0.94	1.35	10	17
1:B:75:VAL:HG22	1:B:86:GLU:HB2	0.94	1.32	20	4
1:B:74:GLU:HB3	1:B:87:VAL:HG13	0.94	1.35	19	1
1:B:102:ARG:CB	1:B:109:LEU:HB3	0.94	1.93	17	1
1:B:87:VAL:HA	1:B:98:ILE:HG23	0.93	1.34	18	7
1:B:19:ALA:HB3	1:B:112:MET:HB2	0.93	1.39	12	7
1:B:19:ALA:HB3	1:B:112:MET:HB3	0.92	1.40	1	7
1:B:99:TYR:HD2	1:B:112:MET:HB2	0.91	1.19	18	1
1:B:96:ALA:HB3	1:B:115:TYR:CZ	0.91	2.01	18	20
1:B:13:TRP:HZ3	1:B:117:ARG:HG2	0.90	1.26	17	1
1:B:31:LYS:HA	1:B:31:LYS:CE	0.90	1.95	10	10
1:B:84:LYS:HE2	1:B:101:THR:OG1	0.89	1.65	17	1
1:B:66:PHE:CD1	1:B:78:SER:HB3	0.89	2.02	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:SER:HB2	1:B:26:LEU:HD23	0.89	1.44	20	16
1:B:22:THR:O	1:B:26:LEU:HG	0.89	1.68	20	5
1:B:17:ALA:CB	1:B:114:LEU:HB3	0.88	1.96	11	19
1:B:40:SER:HB2	1:B:48:LYS:HB3	0.88	1.42	16	1
1:B:83:LYS:HB3	1:B:102:ARG:CZ	0.88	1.99	11	3
1:B:83:LYS:HD2	2:B:158:EB4:C8	0.88	1.99	9	1
1:B:87:VAL:HG23	1:B:98:ILE:CD1	0.87	2.00	18	17
1:B:86:GLU:HG3	1:B:99:TYR:HB3	0.87	1.46	5	6
1:B:102:ARG:HB3	1:B:109:LEU:HB2	0.86	1.44	19	1
1:B:87:VAL:HG23	1:B:98:ILE:HD12	0.86	1.47	18	4
1:B:39:ILE:HD12	1:B:49:VAL:HG12	0.86	1.46	5	17
1:B:129:PHE:CE1	1:B:143:VAL:HG11	0.85	2.07	20	1
1:B:18:LEU:HB2	1:B:144:ALA:HB3	0.85	1.45	13	13
1:B:15:VAL:HG13	1:B:35:ALA:C	0.85	1.97	16	1
1:B:23:GLU:HA	1:B:26:LEU:CD1	0.84	2.01	18	2
1:B:49:VAL:CG2	1:B:64:THR:HB	0.84	2.03	13	2
1:B:87:VAL:CA	1:B:98:ILE:HG23	0.84	2.02	18	2
1:B:75:VAL:HG13	1:B:85:VAL:O	0.84	1.71	17	17
1:B:31:LYS:HA	1:B:31:LYS:NZ	0.83	1.88	3	7
1:B:104:LYS:HD2	1:B:105:ASP:N	0.83	1.86	16	2
1:B:75:VAL:HG22	1:B:86:GLU:CB	0.82	2.04	20	6
1:B:34:MET:HA	1:B:146:LEU:HG	0.82	1.51	9	6
1:B:81:ALA:HB3	1:B:83:LYS:HE3	0.82	1.49	20	3
1:B:17:ALA:HB3	1:B:114:LEU:CB	0.82	2.04	3	19
1:B:70:SER:HA	1:B:75:VAL:O	0.82	1.73	19	1
1:B:91:ASP:HB3	1:B:94:SER:HB3	0.82	1.51	12	17
1:B:15:VAL:HG21	1:B:113:ARG:HG3	0.82	1.51	19	1
1:B:129:PHE:HE1	1:B:143:VAL:HG11	0.82	1.31	20	1
1:B:32:MET:O	1:B:33:LYS:HG3	0.81	1.74	15	2
1:B:91:ASP:CB	1:B:94:SER:HB3	0.81	2.06	12	20
1:B:102:ARG:HD3	2:B:158:EB4:C10	0.81	2.05	11	6
1:B:81:ALA:O	1:B:83:LYS:HG3	0.81	1.74	3	3
1:B:102:ARG:HB2	1:B:102:ARG:NH1	0.81	1.90	14	1
1:B:97:VAL:HG12	1:B:114:LEU:HB2	0.81	1.49	18	1
1:B:18:LEU:HD23	1:B:113:ARG:HG2	0.81	1.52	10	3
1:B:102:ARG:CB	1:B:109:LEU:CB	0.80	2.57	19	2
1:B:55:LYS:HG2	1:B:56:PRO:HD2	0.80	1.54	1	10
1:B:15:VAL:CG1	1:B:35:ALA:HB3	0.80	2.07	19	18
1:B:84:LYS:HE3	1:B:101:THR:CB	0.80	2.06	20	2
1:B:20:SER:HB2	1:B:26:LEU:CD2	0.80	2.07	9	15
1:B:114:LEU:HD11	1:B:125:ALA:HB1	0.80	1.53	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:84:LYS:CG	1:B:101:THR:HG22	0.80	2.07	5	1
1:B:55:LYS:HE3	1:B:57:ASN:OD1	0.79	1.77	8	10
1:B:102:ARG:CG	1:B:109:LEU:HB3	0.79	2.07	15	5
1:B:29:LYS:HA	1:B:29:LYS:CE	0.79	2.06	13	8
1:B:60:ARG:NE	1:B:60:ARG:HA	0.79	1.93	5	8
1:B:77:TYR:CE2	1:B:84:LYS:HE3	0.79	2.13	18	1
1:B:82:LYS:HB3	1:B:103:VAL:CG1	0.78	2.08	17	1
1:B:36:MET:HE1	1:B:153:THR:HG22	0.78	1.55	12	6
1:B:24:PHE:O	1:B:28:GLU:HG2	0.78	1.78	20	8
1:B:13:TRP:CZ3	1:B:117:ARG:HG2	0.78	2.12	17	2
1:B:88:LEU:HD12	1:B:112:MET:HE1	0.78	1.56	4	2
1:B:25:PHE:O	1:B:29:LYS:HG2	0.78	1.79	15	1
1:B:83:LYS:HG2	1:B:102:ARG:CG	0.78	2.08	7	4
1:B:101:THR:C	1:B:102:ARG:HD2	0.78	2.04	18	3
1:B:15:VAL:HG12	1:B:35:ALA:C	0.78	2.04	9	15
1:B:34:MET:CA	1:B:146:LEU:HG	0.77	2.09	9	13
1:B:36:MET:CB	1:B:52:ALA:HB3	0.77	2.06	16	13
1:B:26:LEU:CD2	1:B:142:MET:HA	0.77	2.09	19	9
1:B:15:VAL:CG2	1:B:35:ALA:HB3	0.77	2.10	16	1
1:B:118:SER:HB3	1:B:119:PRO:HD2	0.77	1.55	10	14
1:B:96:ALA:HB3	1:B:115:TYR:CE2	0.77	2.14	17	10
1:B:81:ALA:HB1	1:B:83:LYS:CE	0.77	2.10	9	8
1:B:83:LYS:CG	1:B:102:ARG:HG2	0.76	2.10	16	2
1:B:26:LEU:HD13	1:B:142:MET:HA	0.76	1.56	5	5
1:B:103:VAL:CG2	1:B:108:THR:HG23	0.76	2.09	4	7
1:B:86:GLU:HG2	1:B:99:TYR:HB3	0.76	1.57	11	7
1:B:77:TYR:CE2	1:B:84:LYS:HD2	0.76	2.16	8	2
1:B:83:LYS:HG2	1:B:102:ARG:HG2	0.75	1.57	14	2
1:B:15:VAL:O	1:B:34:MET:HG3	0.75	1.80	14	15
1:B:111:MET:HB2	2:B:158:EB4:C10	0.75	2.12	18	2
1:B:21:ASN:HB3	1:B:109:LEU:HD12	0.75	1.59	20	3
1:B:102:ARG:HB3	1:B:109:LEU:CB	0.75	2.12	19	1
1:B:102:ARG:CD	2:B:158:EB4:C13	0.75	2.60	10	15
1:B:102:ARG:HD3	2:B:158:EB4:H13	0.74	1.59	2	3
1:B:32:MET:HE1	1:B:56:PRO:HD3	0.74	1.59	20	3
1:B:18:LEU:HD13	1:B:29:LYS:CD	0.74	2.13	3	11
1:B:18:LEU:HD23	1:B:113:ARG:HB3	0.74	1.56	8	2
1:B:39:ILE:HD12	1:B:49:VAL:CG1	0.74	2.13	9	16
1:B:83:LYS:HE3	2:B:158:EB4:C8	0.74	2.12	1	1
1:B:47:LEU:HG	1:B:66:PHE:HB2	0.74	1.60	13	7
1:B:42:LEU:CD2	1:B:48:LYS:HB2	0.74	2.13	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:84:LYS:HE2	1:B:86:GLU:HB3	0.74	1.58	7	1
1:B:85:VAL:HG12	1:B:100:ALA:HB1	0.73	1.58	18	2
1:B:16:VAL:HG12	1:B:34:MET:SD	0.73	2.23	2	17
1:B:19:ALA:CB	1:B:112:MET:HB3	0.73	2.14	20	4
1:B:21:ASN:HB2	1:B:110:HIS:HB2	0.73	1.58	7	2
1:B:97:VAL:HG12	1:B:114:LEU:CB	0.73	2.12	18	1
1:B:111:MET:HB2	2:B:158:EB4:C7	0.73	2.13	18	1
1:B:96:ALA:HB3	1:B:115:TYR:CE1	0.73	2.17	18	10
1:B:103:VAL:CG1	1:B:108:THR:HG23	0.73	2.12	3	1
1:B:87:VAL:HA	1:B:98:ILE:HD12	0.72	1.61	20	3
1:B:99:TYR:HD1	1:B:112:MET:HG2	0.72	1.44	2	1
1:B:95:TYR:OH	1:B:128:ILE:HG13	0.72	1.84	6	11
1:B:15:VAL:HG21	1:B:113:ARG:CG	0.72	2.13	19	2
1:B:19:ALA:CB	1:B:112:MET:HB2	0.72	2.15	12	2
1:B:32:MET:HA	1:B:32:MET:HE2	0.72	1.60	11	2
1:B:97:VAL:HB	1:B:112:MET:HE3	0.72	1.61	18	2
1:B:83:LYS:CG	1:B:102:ARG:HG3	0.71	2.13	7	2
1:B:23:GLU:HA	1:B:26:LEU:HD12	0.71	1.59	20	3
1:B:77:TYR:CE1	1:B:84:LYS:HD2	0.71	2.21	17	1
1:B:34:MET:N	1:B:146:LEU:HG	0.71	2.00	2	14
1:B:102:ARG:CD	2:B:158:EB4:H13	0.71	2.16	6	5
1:B:19:ALA:CB	1:B:143:VAL:HG22	0.71	2.15	18	3
1:B:71:ASP:H	1:B:75:VAL:HB	0.71	1.44	13	4
1:B:83:LYS:HB3	1:B:102:ARG:HG3	0.71	1.61	10	1
1:B:15:VAL:HG22	1:B:17:ALA:O	0.71	1.85	19	1
1:B:96:ALA:CB	1:B:115:TYR:CZ	0.71	2.74	19	12
1:B:82:LYS:O	1:B:102:ARG:HB3	0.71	1.86	16	2
1:B:102:ARG:CZ	2:B:158:EB4:C13	0.70	2.68	14	2
1:B:102:ARG:HB2	1:B:109:LEU:CB	0.70	2.08	17	2
1:B:36:MET:HE3	1:B:153:THR:HG22	0.70	1.64	16	1
1:B:84:LYS:HG3	1:B:101:THR:OG1	0.70	1.84	17	1
1:B:34:MET:CG	1:B:146:LEU:HB2	0.70	2.12	16	1
1:B:84:LYS:CG	1:B:101:THR:CB	0.70	2.56	17	1
1:B:18:LEU:CD2	1:B:113:ARG:HD2	0.70	2.17	17	2
1:B:111:MET:HG2	1:B:113:ARG:HD2	0.70	1.63	10	1
1:B:126:THR:HG23	1:B:145:MET:HE1	0.70	1.62	16	4
1:B:87:VAL:CG2	1:B:98:ILE:HD12	0.70	2.15	18	2
1:B:36:MET:HE3	1:B:153:THR:HA	0.70	1.62	18	12
1:B:34:MET:HB2	1:B:146:LEU:HB2	0.69	1.64	19	4
1:B:49:VAL:HG22	1:B:64:THR:HB	0.69	1.61	12	2
1:B:114:LEU:HD12	1:B:129:PHE:HB2	0.69	1.62	20	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:18:LEU:HA	1:B:113:ARG:HG3	0.69	1.64	10	1
1:B:104:LYS:HD3	1:B:105:ASP:N	0.69	2.02	1	6
1:B:51:TYR:HE1	2:B:158:EB4:C6	0.69	2.00	7	3
1:B:88:LEU:HD12	1:B:112:MET:CE	0.69	2.17	18	4
1:B:102:ARG:NH1	1:B:109:LEU:HB3	0.69	2.02	16	3
1:B:102:ARG:CD	2:B:158:EB4:C10	0.69	2.71	15	8
1:B:47:LEU:O	1:B:65:THR:HA	0.69	1.86	20	6
1:B:84:LYS:HG3	1:B:101:THR:HG22	0.69	1.64	5	1
1:B:25:PHE:CZ	1:B:111:MET:HE1	0.69	2.21	13	1
1:B:20:SER:O	1:B:26:LEU:HD21	0.69	1.87	14	17
1:B:29:LYS:HE3	1:B:29:LYS:CA	0.69	2.18	15	10
1:B:19:ALA:HB2	1:B:143:VAL:HA	0.69	1.63	19	1
1:B:102:ARG:HG2	1:B:109:LEU:CB	0.69	2.16	18	1
1:B:38:ARG:HB3	1:B:50:SER:OG	0.68	1.88	20	8
1:B:42:LEU:HD23	1:B:48:LYS:HB2	0.68	1.65	16	2
1:B:18:LEU:HD23	1:B:113:ARG:HG3	0.68	1.64	14	6
1:B:75:VAL:HG22	1:B:86:GLU:HA	0.68	1.65	3	6
1:B:64:THR:HG21	2:B:158:EB4:H11	0.68	1.64	9	7
1:B:79:GLU:O	1:B:82:LYS:HE2	0.68	1.88	13	1
1:B:78:SER:HB2	1:B:81:ALA:HB3	0.68	1.65	9	1
1:B:16:VAL:HG11	1:B:120:GLU:O	0.68	1.89	10	3
1:B:33:LYS:HE2	1:B:149:GLN:OE1	0.68	1.88	12	12
1:B:102:ARG:HB2	1:B:109:LEU:HB2	0.68	1.61	19	1
1:B:94:SER:O	1:B:117:ARG:HG3	0.67	1.90	2	4
1:B:86:GLU:CG	1:B:99:TYR:HB3	0.67	2.19	3	8
1:B:84:LYS:HD2	1:B:101:THR:HB	0.67	1.64	3	3
1:B:87:VAL:CA	1:B:98:ILE:HD12	0.67	2.19	20	2
1:B:148:ARG:O	1:B:148:ARG:HG2	0.67	1.89	10	20
1:B:15:VAL:HG11	1:B:35:ALA:HB3	0.67	1.65	19	11
1:B:114:LEU:HD21	1:B:125:ALA:HB1	0.67	1.64	9	2
1:B:111:MET:HB3	2:B:158:EB4:C10	0.67	2.20	7	2
1:B:26:LEU:O	1:B:30:ASP:HB3	0.67	1.89	14	1
1:B:109:LEU:HD23	2:B:158:EB4:H13	0.67	1.67	17	2
1:B:84:LYS:CE	1:B:101:THR:OG1	0.67	2.43	17	1
1:B:12:LYS:HE3	1:B:156:GLU:CD	0.67	2.15	18	1
1:B:111:MET:HB3	1:B:113:ARG:NH2	0.66	2.05	19	2
1:B:83:LYS:CB	1:B:102:ARG:HG2	0.66	2.19	14	2
1:B:19:ALA:O	1:B:111:MET:HG3	0.66	1.90	20	2
1:B:124:ALA:O	1:B:128:ILE:HG12	0.66	1.90	9	11
1:B:83:LYS:HG2	1:B:102:ARG:HD2	0.66	1.66	19	2
1:B:36:MET:CE	1:B:153:THR:HG22	0.66	2.21	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:TYR:HB3	1:B:125:ALA:HB2	0.66	1.68	9	4
1:B:15:VAL:HG22	1:B:35:ALA:HB3	0.66	1.68	16	1
1:B:129:PHE:HE2	1:B:143:VAL:HG11	0.66	1.50	18	1
1:B:36:MET:CE	1:B:153:THR:HA	0.65	2.21	20	1
1:B:127:ALA:O	1:B:131:LYS:HG3	0.65	1.92	4	14
1:B:102:ARG:HB2	1:B:102:ARG:CZ	0.65	2.19	14	2
1:B:33:LYS:HB2	1:B:54:PRO:HG2	0.65	1.67	17	2
1:B:103:VAL:HG22	1:B:108:THR:CG2	0.65	2.21	16	6
1:B:20:SER:O	1:B:142:MET:HG3	0.65	1.91	19	4
1:B:69:THR:HB	1:B:77:TYR:HD2	0.65	1.50	19	2
1:B:84:LYS:HD2	1:B:85:VAL:N	0.65	2.07	19	1
1:B:18:LEU:CD1	1:B:29:LYS:HD3	0.65	2.22	14	6
1:B:97:VAL:HG13	1:B:114:LEU:HD13	0.65	1.69	18	1
1:B:5:ASP:OD1	1:B:6:ARG:HD3	0.65	1.92	3	2
1:B:111:MET:SD	2:B:158:EB4:C7	0.65	2.85	14	6
1:B:97:VAL:CG1	1:B:114:LEU:HB2	0.65	2.21	18	1
1:B:81:ALA:HB1	1:B:83:LYS:HE2	0.64	1.69	1	2
1:B:46:GLU:HG2	1:B:65:THR:HG22	0.64	1.66	16	2
1:B:13:TRP:N	1:B:13:TRP:CD1	0.64	2.63	20	2
1:B:6:ARG:HB3	1:B:41:PHE:CZ	0.64	2.27	20	5
1:B:26:LEU:CD1	1:B:142:MET:HA	0.64	2.21	5	9
1:B:102:ARG:HD3	1:B:109:LEU:HD23	0.64	1.68	9	1
1:B:84:LYS:HG2	1:B:101:THR:HB	0.64	1.70	8	2
1:B:95:TYR:CZ	1:B:125:ALA:HA	0.64	2.28	18	5
1:B:133:ALA:HB1	1:B:138:TYR:CG	0.64	2.27	17	9
1:B:83:LYS:HG2	1:B:102:ARG:CD	0.64	2.23	8	2
1:B:83:LYS:HB2	1:B:102:ARG:CZ	0.64	2.21	10	2
1:B:75:VAL:CG2	1:B:86:GLU:HB2	0.64	2.18	18	1
1:B:78:SER:HB2	1:B:83:LYS:CA	0.64	2.23	19	1
1:B:82:LYS:HB3	1:B:103:VAL:HG12	0.64	1.70	17	1
1:B:104:LYS:HD3	1:B:105:ASP:H	0.64	1.50	17	3
1:B:12:LYS:HE3	1:B:156:GLU:OE1	0.64	1.93	14	2
1:B:102:ARG:NH1	1:B:102:ARG:HB2	0.64	2.07	16	1
1:B:23:GLU:HA	1:B:26:LEU:CG	0.64	2.22	18	2
1:B:44:GLU:O	1:B:68:LYS:HE3	0.63	1.93	13	4
1:B:102:ARG:HH12	1:B:109:LEU:HB3	0.63	1.53	16	2
1:B:36:MET:HE1	1:B:153:THR:CG2	0.63	2.23	12	2
1:B:97:VAL:HG12	1:B:114:LEU:HD13	0.63	1.69	11	2
1:B:83:LYS:HD3	1:B:102:ARG:NH2	0.63	2.08	18	1
1:B:102:ARG:HB3	1:B:109:LEU:CG	0.63	2.23	19	1
1:B:21:ASN:OD1	1:B:110:HIS:HB2	0.63	1.93	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:55:LYS:CG	1:B:56:PRO:HD2	0.63	2.23	1	17
1:B:102:ARG:HD2	2:B:158:EB4:C16	0.63	2.23	1	3
1:B:77:TYR:CZ	1:B:84:LYS:HE3	0.63	2.28	18	1
1:B:81:ALA:CB	1:B:83:LYS:HE2	0.63	2.23	1	1
1:B:102:ARG:NE	2:B:158:EB4:C13	0.63	2.62	16	5
1:B:49:VAL:O	1:B:63:GLU:HA	0.63	1.92	3	16
1:B:83:LYS:HB3	1:B:102:ARG:NH1	0.63	2.07	7	2
1:B:97:VAL:CG1	1:B:129:PHE:HD2	0.63	2.06	20	1
1:B:69:THR:HG21	1:B:77:TYR:CD1	0.63	2.28	12	4
1:B:111:MET:HG2	1:B:113:ARG:NH1	0.63	2.09	11	4
1:B:32:MET:O	1:B:33:LYS:CG	0.63	2.47	15	3
1:B:33:LYS:HB2	1:B:54:PRO:CG	0.63	2.23	17	2
1:B:16:VAL:HG22	1:B:114:LEU:O	0.63	1.94	19	1
1:B:18:LEU:HD13	1:B:29:LYS:CE	0.62	2.23	1	2
1:B:51:TYR:O	1:B:61:LYS:HA	0.62	1.93	2	12
1:B:68:LYS:HD3	1:B:76:TYR:CE1	0.62	2.28	5	4
1:B:22:THR:HB	1:B:25:PHE:CD1	0.62	2.29	7	1
1:B:26:LEU:HD13	1:B:141:GLU:O	0.62	1.94	18	3
1:B:91:ASP:CG	1:B:94:SER:HB3	0.62	2.20	9	8
1:B:95:TYR:CD1	1:B:125:ALA:HB2	0.62	2.29	7	3
1:B:17:ALA:HB2	1:B:114:LEU:HB3	0.62	1.69	20	2
1:B:97:VAL:HG11	1:B:129:PHE:CD1	0.62	2.29	18	1
1:B:83:LYS:CB	1:B:102:ARG:HG3	0.62	2.25	10	1
1:B:49:VAL:HG21	1:B:66:PHE:HE2	0.62	1.55	12	1
1:B:66:PHE:CD2	1:B:78:SER:HB3	0.62	2.30	2	1
1:B:20:SER:OG	1:B:111:MET:HE2	0.62	1.94	12	5
1:B:97:VAL:HG11	1:B:129:PHE:HD1	0.62	1.54	18	1
1:B:78:SER:HB2	1:B:83:LYS:C	0.62	2.20	19	1
1:B:96:ALA:O	1:B:114:LEU:HD12	0.61	1.95	9	3
1:B:19:ALA:CB	1:B:143:VAL:HA	0.61	2.24	19	1
1:B:84:LYS:CD	1:B:101:THR:HB	0.61	2.25	3	2
1:B:100:ALA:HB3	1:B:111:MET:O	0.61	1.96	8	4
1:B:78:SER:HB2	1:B:83:LYS:HG3	0.61	1.72	10	2
1:B:102:ARG:HD3	2:B:158:EB4:C16	0.61	2.24	10	1
1:B:12:LYS:HD3	1:B:156:GLU:HB3	0.61	1.73	3	2
1:B:102:ARG:CD	2:B:158:EB4:O7	0.61	2.48	1	3
1:B:88:LEU:HD12	1:B:112:MET:HE3	0.61	1.73	3	4
1:B:22:THR:HG23	1:B:109:LEU:HD13	0.61	1.72	14	1
1:B:18:LEU:HD23	1:B:113:ARG:HD2	0.61	1.72	16	1
1:B:25:PHE:CZ	1:B:109:LEU:HD21	0.61	2.30	18	1
1:B:95:TYR:CB	1:B:125:ALA:HB2	0.61	2.26	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:87:VAL:CB	1:B:98:ILE:HD12	0.61	2.26	18	2
1:B:145:MET:C	1:B:146:LEU:HD22	0.60	2.21	16	13
1:B:95:TYR:OH	1:B:128:ILE:HG21	0.60	1.96	4	2
1:B:97:VAL:CG1	1:B:114:LEU:HD13	0.60	2.25	11	2
1:B:34:MET:HB2	1:B:146:LEU:CB	0.60	2.26	9	10
1:B:96:ALA:CB	1:B:115:TYR:CE2	0.60	2.83	19	4
1:B:46:GLU:CG	1:B:65:THR:HG22	0.60	2.25	16	4
1:B:36:MET:HB2	1:B:52:ALA:CB	0.60	2.14	16	2
1:B:82:LYS:HE3	1:B:82:LYS:HA	0.60	1.73	12	1
1:B:87:VAL:N	1:B:98:ILE:HG23	0.60	2.11	20	2
1:B:35:ALA:CB	1:B:53:VAL:HG12	0.60	2.26	2	10
1:B:19:ALA:O	1:B:111:MET:HA	0.60	1.96	11	5
1:B:69:THR:HG21	1:B:77:TYR:CG	0.60	2.31	18	1
1:B:47:LEU:CG	1:B:66:PHE:HB2	0.60	2.26	13	4
1:B:95:TYR:CG	1:B:125:ALA:HB2	0.60	2.32	13	8
1:B:112:MET:HB3	1:B:129:PHE:CZ	0.60	2.32	12	1
1:B:16:VAL:HA	1:B:34:MET:HG2	0.60	1.72	16	1
1:B:89:ASP:HB3	1:B:97:VAL:HG22	0.60	1.71	19	1
1:B:83:LYS:NZ	2:B:158:EB4:C14	0.60	2.65	13	20
1:B:39:ILE:HG23	1:B:49:VAL:CG1	0.60	2.22	9	3
1:B:101:THR:HG23	1:B:109:LEU:O	0.60	1.97	18	1
1:B:45:ASP:HA	1:B:68:LYS:CB	0.59	2.27	13	2
1:B:29:LYS:HE3	1:B:32:MET:HG3	0.59	1.74	15	1
1:B:18:LEU:HD23	1:B:113:ARG:CG	0.59	2.26	10	4
1:B:28:GLU:O	1:B:32:MET:HG2	0.59	1.97	15	7
1:B:133:ALA:O	1:B:138:TYR:HB3	0.59	1.96	8	15
1:B:70:SER:HB3	1:B:73:GLY:O	0.59	1.96	5	3
1:B:19:ALA:HB3	1:B:112:MET:O	0.59	1.98	18	1
1:B:51:TYR:CE1	2:B:158:EB4:C6	0.59	2.85	7	4
1:B:69:THR:OG1	1:B:77:TYR:HB2	0.59	1.98	18	5
1:B:68:LYS:HA	1:B:76:TYR:CD2	0.59	2.33	7	1
1:B:26:LEU:HD22	1:B:142:MET:CA	0.59	2.13	19	2
1:B:81:ALA:HB1	1:B:83:LYS:CD	0.59	2.28	16	1
1:B:23:GLU:HA	1:B:26:LEU:HG	0.59	1.72	18	1
1:B:82:LYS:HB2	1:B:104:LYS:NZ	0.59	2.12	10	1
1:B:15:VAL:HG21	1:B:113:ARG:HG2	0.59	1.73	1	3
1:B:44:GLU:O	1:B:68:LYS:HE2	0.59	1.97	10	2
1:B:109:LEU:HD23	2:B:158:EB4:O7	0.59	1.98	18	2
1:B:26:LEU:HB3	1:B:141:GLU:O	0.58	1.98	13	13
1:B:51:TYR:CE2	2:B:158:EB4:C2	0.58	2.86	9	3
1:B:33:LYS:HG2	1:B:149:GLN:CD	0.58	2.22	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:83:LYS:HD2	2:B:158:EB4:H8	0.58	1.70	9	1
1:B:95:TYR:CZ	1:B:128:ILE:HG13	0.58	2.33	9	3
1:B:66:PHE:HD2	1:B:78:SER:HB3	0.58	1.57	2	1
1:B:84:LYS:HD2	1:B:84:LYS:C	0.58	2.24	20	3
1:B:126:THR:HG23	1:B:145:MET:SD	0.58	2.38	12	7
1:B:82:LYS:C	1:B:83:LYS:HG3	0.58	2.23	19	4
1:B:135:GLU:OE1	1:B:136:ARG:HD2	0.58	1.99	15	1
1:B:84:LYS:CE	1:B:101:THR:HB	0.58	2.19	16	1
1:B:83:LYS:HB3	1:B:102:ARG:NH2	0.58	2.12	2	1
1:B:102:ARG:NE	2:B:158:EB4:C10	0.58	2.66	15	5
1:B:83:LYS:NZ	2:B:158:EB4:C11	0.58	2.67	4	20
1:B:112:MET:O	1:B:113:ARG:HG3	0.58	1.98	7	1
1:B:112:MET:HG2	1:B:129:PHE:CZ	0.58	2.34	17	1
1:B:114:LEU:C	1:B:114:LEU:HD23	0.57	2.24	20	10
1:B:87:VAL:HG23	1:B:98:ILE:HD13	0.57	1.75	19	3
1:B:114:LEU:HD23	1:B:115:TYR:N	0.57	2.14	10	15
1:B:114:LEU:CD1	1:B:125:ALA:HB1	0.57	2.28	10	3
1:B:114:LEU:CD1	1:B:129:PHE:HB2	0.57	2.29	1	3
1:B:126:THR:HG23	1:B:145:MET:CE	0.57	2.28	16	7
1:B:90:THR:OG1	1:B:96:ALA:HB2	0.57	1.98	20	14
1:B:17:ALA:O	1:B:18:LEU:HG	0.57	1.99	16	2
1:B:102:ARG:CA	1:B:109:LEU:HB2	0.57	2.27	19	1
1:B:4:PRO:HA	1:B:7:SER:OG	0.57	2.00	8	1
1:B:102:ARG:HB3	1:B:102:ARG:CZ	0.57	2.29	15	1
1:B:121:VAL:HG21	1:B:146:LEU:O	0.56	2.00	16	6
1:B:102:ARG:HD2	1:B:102:ARG:N	0.56	2.15	18	2
1:B:102:ARG:HB3	1:B:109:LEU:HD23	0.56	1.77	19	1
1:B:69:THR:O	1:B:75:VAL:HB	0.56	2.01	16	4
1:B:78:SER:CB	1:B:83:LYS:HB2	0.56	2.30	19	1
1:B:53:VAL:HG11	2:B:158:EB4:O9	0.56	2.01	15	1
1:B:86:GLU:HG2	1:B:99:TYR:O	0.56	2.00	19	1
1:B:19:ALA:HB3	1:B:112:MET:CB	0.56	2.29	4	5
1:B:134:GLY:HA2	1:B:138:TYR:CD1	0.56	2.35	9	6
1:B:12:LYS:HE2	1:B:156:GLU:OE2	0.56	2.00	11	4
1:B:82:LYS:HB3	1:B:103:VAL:HG13	0.56	1.75	17	1
1:B:18:LEU:HD22	1:B:113:ARG:HD2	0.56	1.75	17	1
1:B:62:TRP:HA	1:B:62:TRP:CE3	0.56	2.36	19	2
1:B:83:LYS:CD	2:B:158:EB4:C8	0.56	2.80	9	1
1:B:46:GLU:HA	1:B:66:PHE:O	0.56	2.01	16	1
1:B:42:LEU:HB3	1:B:46:GLU:HG2	0.56	1.78	2	6
1:B:21:ASN:CB	1:B:110:HIS:HB2	0.56	2.30	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:85:VAL:HG12	1:B:100:ALA:HB2	0.56	1.76	18	1
1:B:98:ILE:HG12	1:B:115:TYR:HE2	0.56	1.61	18	1
1:B:102:ARG:O	1:B:109:LEU:N	0.56	2.35	18	1
1:B:18:LEU:O	1:B:143:VAL:HG13	0.55	2.00	18	1
1:B:51:TYR:CZ	2:B:158:EB4:O6	0.55	2.59	10	5
1:B:112:MET:HE3	1:B:129:PHE:CZ	0.55	2.36	13	3
1:B:97:VAL:HG11	1:B:129:PHE:HD2	0.55	1.61	20	1
1:B:77:TYR:CZ	1:B:84:LYS:HD3	0.55	2.36	4	1
1:B:100:ALA:O	1:B:111:MET:N	0.55	2.39	20	2
1:B:139:THR:OG1	1:B:142:MET:HB2	0.55	2.02	20	1
1:B:84:LYS:HD2	1:B:101:THR:CB	0.55	2.31	3	1
1:B:111:MET:HG2	1:B:113:ARG:HH11	0.55	1.62	7	2
1:B:45:ASP:OD1	1:B:68:LYS:HB3	0.55	2.02	4	6
1:B:81:ALA:CB	1:B:83:LYS:HD3	0.55	2.31	16	1
1:B:69:THR:HB	1:B:77:TYR:HD1	0.55	1.61	13	2
1:B:46:GLU:HG2	1:B:65:THR:CG2	0.55	2.31	16	2
1:B:75:VAL:HG13	1:B:86:GLU:HB3	0.55	1.78	20	2
1:B:51:TYR:CE2	2:B:158:EB4:C5	0.55	2.90	15	8
1:B:71:ASP:N	1:B:75:VAL:HB	0.55	2.17	13	1
1:B:17:ALA:CB	1:B:114:LEU:CB	0.55	2.82	20	1
1:B:126:THR:CG2	1:B:145:MET:HE1	0.54	2.32	5	7
1:B:78:SER:HB2	1:B:83:LYS:O	0.54	2.02	19	1
1:B:25:PHE:HD2	1:B:111:MET:HE3	0.54	1.63	2	1
1:B:42:LEU:HD13	1:B:42:LEU:O	0.54	2.03	18	6
1:B:86:GLU:C	1:B:98:ILE:HG23	0.54	2.27	20	2
1:B:18:LEU:N	1:B:144:ALA:O	0.54	2.36	19	1
1:B:95:TYR:CD2	1:B:125:ALA:HB2	0.54	2.37	2	5
1:B:42:LEU:HD23	1:B:48:LYS:HE2	0.54	1.78	1	3
1:B:16:VAL:CG1	1:B:121:VAL:HG22	0.54	2.32	20	1
1:B:35:ALA:HB1	1:B:53:VAL:HG12	0.54	1.80	9	6
1:B:114:LEU:HB2	1:B:129:PHE:CD1	0.54	2.38	19	3
1:B:25:PHE:O	1:B:29:LYS:HB2	0.54	2.02	19	5
1:B:41:PHE:N	1:B:41:PHE:CD1	0.54	2.76	16	1
1:B:6:ARG:HB3	1:B:41:PHE:CE2	0.54	2.38	20	2
1:B:82:LYS:O	1:B:83:LYS:HG3	0.54	2.03	19	1
1:B:97:VAL:HG12	1:B:114:LEU:CA	0.54	2.32	18	1
1:B:100:ALA:HB3	2:B:158:EB4:H7	0.54	1.78	18	1
1:B:18:LEU:HD13	1:B:29:LYS:HD2	0.54	1.78	5	2
1:B:34:MET:HB2	1:B:146:LEU:HB3	0.54	1.78	15	3
1:B:15:VAL:CG2	1:B:113:ARG:CG	0.54	2.84	19	2
1:B:102:ARG:HG3	2:B:158:EB4:C10	0.54	2.33	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:SER:HA	1:B:62:TRP:O	0.53	2.02	18	3
1:B:30:ASP:OD1	1:B:31:LYS:HE2	0.53	2.03	3	1
1:B:103:VAL:HG22	1:B:108:THR:HG22	0.53	1.79	15	1
1:B:38:ARG:HD2	1:B:50:SER:OG	0.53	2.02	1	3
1:B:111:MET:HG2	1:B:113:ARG:CD	0.53	2.32	10	1
1:B:16:VAL:HG12	1:B:34:MET:CE	0.53	2.33	16	1
1:B:33:LYS:HE3	1:B:149:GLN:OE1	0.53	2.02	20	1
1:B:67:LYS:N	1:B:67:LYS:HD2	0.53	2.18	9	1
1:B:97:VAL:HB	1:B:112:MET:CE	0.53	2.34	14	1
1:B:102:ARG:NH1	1:B:109:LEU:HD23	0.53	2.18	4	1
1:B:21:ASN:O	1:B:21:ASN:ND2	0.53	2.40	16	3
1:B:13:TRP:HB3	1:B:115:TYR:CD2	0.53	2.37	12	3
1:B:99:TYR:OH	1:B:110:HIS:HB3	0.53	2.03	20	3
1:B:130:ARG:HG2	1:B:138:TYR:OH	0.53	2.02	12	3
1:B:83:LYS:HZ2	2:B:158:EB4:C11	0.53	2.17	18	13
1:B:38:ARG:NH1	1:B:156:GLU:HA	0.53	2.18	6	1
1:B:32:MET:CE	1:B:56:PRO:HD3	0.53	2.32	14	1
1:B:29:LYS:CE	1:B:32:MET:HG3	0.53	2.34	15	1
1:B:51:TYR:OH	2:B:158:EB4:O6	0.53	2.26	11	4
1:B:55:LYS:HG3	1:B:56:PRO:HD2	0.53	1.81	9	4
1:B:64:THR:HB	1:B:66:PHE:HE1	0.53	1.63	20	1
1:B:146:LEU:HD22	1:B:146:LEU:N	0.53	2.19	16	17
1:B:88:LEU:HD11	1:B:99:TYR:HB2	0.53	1.80	2	3
1:B:72:ASP:H	1:B:75:VAL:HG21	0.53	1.64	13	1
1:B:102:ARG:O	1:B:108:THR:HG22	0.53	2.04	17	1
1:B:12:LYS:C	1:B:13:TRP:CD1	0.53	2.87	18	2
1:B:147:PRO:O	1:B:149:GLN:N	0.52	2.42	15	13
1:B:51:TYR:HE2	2:B:158:EB4:C2	0.52	2.16	9	1
1:B:19:ALA:HB2	1:B:143:VAL:HG22	0.52	1.80	18	2
1:B:97:VAL:C	1:B:98:ILE:HD13	0.52	2.29	20	2
1:B:111:MET:SD	2:B:158:EB4:C10	0.52	2.97	3	7
1:B:88:LEU:CG	1:B:99:TYR:HB2	0.52	2.34	17	2
1:B:88:LEU:HB2	1:B:97:VAL:HG23	0.52	1.81	13	2
1:B:90:THR:HA	1:B:96:ALA:CB	0.52	2.34	18	2
1:B:47:LEU:HD22	1:B:76:TYR:CD1	0.52	2.39	8	2
1:B:29:LYS:HA	1:B:29:LYS:HE3	0.52	1.79	12	1
1:B:79:GLU:CD	1:B:79:GLU:C	0.52	2.77	19	1
1:B:42:LEU:HD23	1:B:48:LYS:CE	0.52	2.34	2	1
1:B:33:LYS:HG2	1:B:149:GLN:NE2	0.52	2.19	3	1
1:B:14:TYR:CZ	1:B:119:PRO:HD3	0.52	2.40	10	4
1:B:97:VAL:HG12	1:B:114:LEU:HA	0.52	1.81	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:TYR:HB2	1:B:62:TRP:O	0.52	2.05	7	2
1:B:74:GLU:O	1:B:87:VAL:HG12	0.52	2.05	19	1
1:B:13:TRP:CE3	1:B:115:TYR:CE1	0.52	2.98	20	1
1:B:114:LEU:HD12	1:B:129:PHE:CB	0.52	2.35	20	1
1:B:95:TYR:CE1	1:B:128:ILE:HG21	0.52	2.40	9	1
1:B:29:LYS:HA	1:B:29:LYS:HE2	0.52	1.81	16	1
1:B:20:SER:CB	1:B:25:PHE:HB3	0.52	2.35	13	2
1:B:34:MET:CE	1:B:150:GLU:HB3	0.51	2.35	15	2
1:B:34:MET:HE1	1:B:150:GLU:CG	0.51	2.35	15	1
1:B:102:ARG:HB3	1:B:109:LEU:CD2	0.51	2.35	19	1
1:B:78:SER:HB2	1:B:83:LYS:CG	0.51	2.35	10	2
1:B:122:SER:OG	1:B:125:ALA:HB3	0.51	2.04	18	2
1:B:47:LEU:HD13	1:B:76:TYR:CE1	0.51	2.41	17	1
1:B:26:LEU:HD22	1:B:141:GLU:O	0.51	2.05	18	5
1:B:132:LEU:O	1:B:136:ARG:HG3	0.51	2.05	18	3
1:B:51:TYR:HE2	2:B:158:EB4:C8	0.51	2.19	8	1
1:B:32:MET:O	1:B:33:LYS:CB	0.51	2.57	19	2
1:B:102:ARG:HG3	1:B:109:LEU:HB3	0.51	1.83	6	1
1:B:76:TYR:HB2	1:B:85:VAL:CG2	0.51	2.36	9	3
1:B:83:LYS:CE	2:B:158:EB4:C11	0.51	2.88	16	2
1:B:102:ARG:HD2	2:B:158:EB4:O7	0.51	2.05	1	2
1:B:31:LYS:HE2	1:B:31:LYS:CA	0.51	2.26	16	4
1:B:66:PHE:HD1	1:B:78:SER:CB	0.51	2.09	4	1
1:B:22:THR:OG1	1:B:109:LEU:HD11	0.51	2.05	13	1
1:B:32:MET:C	1:B:33:LYS:HG3	0.51	2.31	15	1
1:B:111:MET:SD	2:B:158:EB4:C4	0.51	2.99	18	1
1:B:85:VAL:HG12	1:B:100:ALA:CA	0.51	2.35	20	1
1:B:69:THR:O	1:B:71:ASP:N	0.50	2.43	7	9
1:B:15:VAL:HG13	1:B:15:VAL:O	0.50	2.06	9	4
1:B:84:LYS:HD3	1:B:85:VAL:N	0.50	2.21	7	1
1:B:87:VAL:HG13	1:B:87:VAL:O	0.50	2.06	17	7
1:B:18:LEU:HD23	1:B:113:ARG:CD	0.50	2.35	16	2
1:B:129:PHE:CE2	1:B:143:VAL:HG11	0.50	2.39	18	1
1:B:32:MET:HA	1:B:32:MET:CE	0.50	2.36	20	1
1:B:15:VAL:CG1	1:B:35:ALA:C	0.50	2.84	13	9
1:B:99:TYR:HB2	1:B:112:MET:SD	0.50	2.46	18	1
1:B:45:ASP:HA	1:B:68:LYS:HB2	0.50	1.83	13	1
1:B:28:GLU:O	1:B:32:MET:HG3	0.50	2.07	18	2
1:B:42:LEU:HB2	1:B:46:GLU:O	0.50	2.06	16	1
1:B:84:LYS:CG	1:B:101:THR:OG1	0.50	2.59	17	1
1:B:102:ARG:CZ	2:B:158:EB4:O7	0.50	2.60	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:78:SER:CB	1:B:83:LYS:HG3	0.50	2.36	10	1
1:B:69:THR:HB	1:B:77:TYR:CD1	0.50	2.41	2	3
1:B:130:ARG:HG3	1:B:138:TYR:OH	0.50	2.06	6	5
1:B:15:VAL:HG21	1:B:113:ARG:HB3	0.50	1.82	18	1
1:B:66:PHE:C	1:B:67:LYS:HD2	0.49	2.32	6	4
1:B:55:LYS:HG2	1:B:56:PRO:CD	0.49	2.34	1	4
1:B:96:ALA:O	1:B:114:LEU:HG	0.49	2.07	15	2
1:B:16:VAL:HA	1:B:34:MET:CG	0.49	2.37	16	1
1:B:100:ALA:CB	2:B:158:EB4:H7	0.49	2.36	18	1
1:B:82:LYS:O	1:B:102:ARG:HG3	0.49	2.07	8	1
1:B:19:ALA:HB1	1:B:142:MET:HG2	0.49	1.84	19	1
1:B:114:LEU:HD23	1:B:114:LEU:C	0.49	2.33	12	6
1:B:69:THR:HB	1:B:77:TYR:CD2	0.49	2.37	19	2
1:B:19:ALA:CB	1:B:112:MET:CB	0.49	2.90	20	1
1:B:77:TYR:CD2	1:B:84:LYS:HB3	0.49	2.42	2	2
1:B:51:TYR:OH	2:B:158:EB4:O5	0.49	2.31	11	2
1:B:13:TRP:HE3	1:B:115:TYR:CE1	0.49	2.24	20	1
1:B:31:LYS:HA	1:B:31:LYS:HZ3	0.49	1.60	3	1
1:B:118:SER:HB3	1:B:119:PRO:CD	0.49	2.35	10	1
1:B:49:VAL:CG2	1:B:66:PHE:HE2	0.49	2.19	12	1
1:B:88:LEU:HD21	1:B:99:TYR:HB2	0.49	1.84	12	1
1:B:102:ARG:CZ	1:B:102:ARG:CB	0.49	2.90	15	1
1:B:138:TYR:HB2	1:B:142:MET:SD	0.49	2.47	20	2
1:B:15:VAL:O	1:B:15:VAL:HG13	0.49	2.08	14	12
1:B:52:ALA:CB	1:B:154:VAL:HB	0.49	2.38	9	4
1:B:98:ILE:HG12	1:B:115:TYR:CE2	0.49	2.43	18	1
1:B:49:VAL:HG23	1:B:64:THR:HB	0.49	1.80	13	1
1:B:47:LEU:CD2	1:B:66:PHE:HB2	0.49	2.38	16	1
1:B:81:ALA:CB	1:B:83:LYS:CE	0.49	2.81	20	1
1:B:112:MET:HG2	1:B:129:PHE:CE2	0.49	2.43	13	1
1:B:34:MET:HE1	1:B:150:GLU:HB3	0.49	1.84	18	1
1:B:20:SER:HB3	1:B:25:PHE:HB3	0.49	1.85	19	1
1:B:139:THR:O	1:B:142:MET:HB3	0.49	2.08	13	8
1:B:149:GLN:HG2	1:B:149:GLN:O	0.49	2.07	3	1
1:B:104:LYS:HE2	1:B:104:LYS:HA	0.49	1.84	5	1
1:B:95:TYR:HB2	1:B:114:LEU:HD21	0.49	1.83	15	2
1:B:112:MET:CB	1:B:129:PHE:HZ	0.49	2.21	12	1
1:B:34:MET:HE1	1:B:150:GLU:HG3	0.49	1.85	15	1
1:B:148:ARG:O	1:B:148:ARG:CG	0.48	2.60	10	7
1:B:83:LYS:HB3	1:B:102:ARG:CG	0.48	2.36	10	1
1:B:97:VAL:HG12	1:B:114:LEU:CG	0.48	2.38	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:36:MET:HE3	1:B:152:CYS:O	0.48	2.08	10	9
1:B:42:LEU:HD13	1:B:42:LEU:C	0.48	2.33	19	8
1:B:15:VAL:CG2	1:B:113:ARG:HG2	0.48	2.38	4	3
1:B:114:LEU:HB2	1:B:129:PHE:CD2	0.48	2.43	20	2
1:B:78:SER:HB2	1:B:83:LYS:HB2	0.48	1.85	19	2
1:B:82:LYS:CB	1:B:103:VAL:CG1	0.48	2.90	17	1
1:B:85:VAL:CG1	1:B:100:ALA:CB	0.48	2.80	18	2
1:B:84:LYS:NZ	1:B:101:THR:OG1	0.48	2.40	19	1
1:B:111:MET:HB3	1:B:113:ARG:NH1	0.48	2.24	1	2
1:B:23:GLU:CA	1:B:26:LEU:HG	0.48	2.37	18	1
1:B:133:ALA:HB1	1:B:138:TYR:CD2	0.48	2.44	9	4
1:B:109:LEU:CD2	1:B:111:MET:HE3	0.48	2.39	13	1
1:B:83:LYS:HZ3	2:B:158:EB4:C14	0.48	2.21	16	1
1:B:104:LYS:HD2	1:B:105:ASP:H	0.48	1.64	16	1
1:B:74:GLU:CB	1:B:87:VAL:HG13	0.48	2.24	19	1
1:B:102:ARG:N	1:B:109:LEU:O	0.48	2.42	20	1
1:B:112:MET:HB3	1:B:129:PHE:HZ	0.48	1.68	12	1
1:B:150:GLU:CD	1:B:150:GLU:C	0.48	2.81	20	1
1:B:42:LEU:H	1:B:47:LEU:HA	0.48	1.66	12	1
1:B:16:VAL:CG2	1:B:121:VAL:HG22	0.48	2.38	14	1
1:B:79:GLU:O	1:B:82:LYS:HD3	0.48	2.08	10	2
1:B:97:VAL:HG12	1:B:114:LEU:HG	0.48	1.84	20	1
1:B:100:ALA:HB3	1:B:111:MET:HB3	0.48	1.85	17	1
1:B:84:LYS:HE2	1:B:86:GLU:CD	0.48	2.34	1	1
1:B:95:TYR:CG	1:B:125:ALA:CB	0.48	2.96	20	2
1:B:19:ALA:O	1:B:111:MET:HG2	0.48	2.08	4	1
1:B:38:ARG:HB3	1:B:50:SER:HG	0.48	1.69	4	1
1:B:77:TYR:CZ	1:B:84:LYS:CG	0.48	2.97	7	1
1:B:17:ALA:HB3	1:B:114:LEU:H	0.48	1.68	18	1
1:B:19:ALA:HB3	1:B:112:MET:CA	0.48	2.38	20	1
1:B:126:THR:HG21	1:B:145:MET:SD	0.48	2.48	20	1
1:B:21:ASN:O	1:B:22:THR:HG23	0.47	2.09	10	1
1:B:150:GLU:O	1:B:151:GLU:CB	0.47	2.62	20	1
1:B:82:LYS:CB	1:B:103:VAL:HG12	0.47	2.39	17	1
1:B:104:LYS:HB2	1:B:107:ARG:O	0.47	2.09	19	1
1:B:68:LYS:HD2	1:B:70:SER:OG	0.47	2.09	3	2
1:B:45:ASP:O	1:B:67:LYS:HA	0.47	2.09	5	1
1:B:17:ALA:HB3	1:B:114:LEU:N	0.47	2.24	18	1
1:B:88:LEU:HD12	1:B:112:MET:SD	0.47	2.49	18	1
1:B:90:THR:HA	1:B:96:ALA:HB2	0.47	1.86	18	1
1:B:31:LYS:CE	1:B:31:LYS:CA	0.47	2.89	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:VAL:HG23	1:B:60:ARG:HB3	0.47	1.86	8	1
1:B:18:LEU:HD13	1:B:29:LYS:HE2	0.47	1.86	1	2
1:B:19:ALA:O	1:B:111:MET:HB2	0.47	2.09	14	2
1:B:102:ARG:NH1	2:B:158:EB4:O7	0.47	2.48	20	2
1:B:78:SER:HB3	1:B:81:ALA:HB3	0.47	1.85	19	1
1:B:109:LEU:N	1:B:109:LEU:HD12	0.47	2.25	7	1
1:B:75:VAL:CG2	1:B:86:GLU:CB	0.47	2.87	20	2
1:B:38:ARG:HD3	1:B:50:SER:OG	0.47	2.10	19	1
1:B:101:THR:O	1:B:102:ARG:HG3	0.47	2.09	14	1
1:B:138:TYR:CD2	1:B:143:VAL:HG21	0.47	2.45	19	1
1:B:30:ASP:OD2	1:B:31:LYS:HE2	0.47	2.09	19	2
1:B:75:VAL:HG11	1:B:84:LYS:HE3	0.47	1.85	7	1
1:B:88:LEU:HG	1:B:99:TYR:HB2	0.47	1.87	17	1
1:B:38:ARG:HB3	1:B:50:SER:HB2	0.47	1.87	19	1
1:B:22:THR:O	1:B:26:LEU:CG	0.46	2.58	18	1
1:B:15:VAL:HG11	2:B:158:EB4:H12	0.46	1.86	9	2
1:B:96:ALA:CB	1:B:115:TYR:CE1	0.46	2.99	14	1
1:B:13:TRP:N	1:B:13:TRP:HD1	0.46	2.09	20	1
1:B:66:PHE:O	1:B:67:LYS:HE3	0.46	2.10	20	1
1:B:33:LYS:HG2	1:B:149:GLN:OE1	0.46	2.09	5	4
1:B:83:LYS:HD3	2:B:158:EB4:C8	0.46	2.40	10	1
1:B:86:GLU:HG3	1:B:99:TYR:HD2	0.46	1.70	9	2
1:B:12:LYS:HE2	1:B:156:GLU:CD	0.46	2.36	11	1
1:B:103:VAL:HB	1:B:108:THR:HG23	0.46	1.87	11	1
1:B:25:PHE:CE2	1:B:111:MET:HE1	0.46	2.45	13	1
1:B:15:VAL:HA	1:B:115:TYR:HA	0.46	1.85	19	1
1:B:78:SER:HB2	1:B:83:LYS:CB	0.46	2.41	19	1
1:B:42:LEU:CB	1:B:46:GLU:HG2	0.46	2.41	8	2
1:B:67:LYS:HD2	1:B:67:LYS:N	0.46	2.26	18	2
1:B:77:TYR:CE2	1:B:84:LYS:HE2	0.46	2.45	6	1
1:B:100:ALA:HB1	1:B:102:ARG:NH1	0.46	2.24	10	1
1:B:42:LEU:HD12	1:B:46:GLU:HG2	0.46	1.88	11	1
1:B:101:THR:O	1:B:102:ARG:HD2	0.46	2.11	11	1
1:B:136:ARG:O	1:B:137:ASN:HB2	0.46	2.11	18	2
1:B:9:ILE:O	1:B:9:ILE:HG22	0.46	2.11	20	8
1:B:81:ALA:O	1:B:83:LYS:HD3	0.46	2.11	1	1
1:B:36:MET:SD	1:B:154:VAL:HG12	0.46	2.51	5	1
1:B:13:TRP:HB3	1:B:115:TYR:CD1	0.46	2.45	10	1
1:B:75:VAL:HG12	1:B:76:TYR:N	0.46	2.25	13	11
1:B:112:MET:HG3	1:B:129:PHE:CE1	0.46	2.46	1	1
1:B:150:GLU:H	1:B:150:GLU:CD	0.46	2.14	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:93:LYS:C	1:B:117:ARG:HD3	0.46	2.35	16	1
1:B:102:ARG:CD	1:B:102:ARG:N	0.46	2.79	18	1
1:B:15:VAL:HG13	1:B:35:ALA:O	0.46	2.10	16	1
1:B:46:GLU:CG	1:B:65:THR:CG2	0.46	2.93	16	1
1:B:14:TYR:HE2	1:B:119:PRO:HD3	0.46	1.71	18	1
1:B:29:LYS:HE3	1:B:29:LYS:O	0.46	2.11	20	1
1:B:109:LEU:HD21	1:B:111:MET:HE3	0.45	1.88	13	1
1:B:103:VAL:HA	1:B:108:THR:HG22	0.45	1.86	15	1
1:B:14:TYR:CE1	1:B:153:THR:HG22	0.45	2.45	20	1
1:B:138:TYR:CD2	1:B:143:VAL:CG2	0.45	2.99	19	2
1:B:75:VAL:CG1	1:B:76:TYR:N	0.45	2.79	3	11
1:B:104:LYS:O	1:B:105:ASP:C	0.45	2.60	16	7
1:B:51:TYR:N	1:B:62:TRP:O	0.45	2.47	7	1
1:B:69:THR:CG2	1:B:77:TYR:CD1	0.45	2.98	12	1
1:B:51:TYR:HE1	2:B:158:EB4:C3	0.45	2.24	7	1
1:B:6:ARG:N	1:B:6:ARG:HD3	0.45	2.26	11	1
1:B:15:VAL:CG2	1:B:113:ARG:HB3	0.45	2.42	18	1
1:B:63:GLU:CD	1:B:63:GLU:N	0.45	2.74	19	1
1:B:97:VAL:O	1:B:97:VAL:HG23	0.45	2.11	20	1
1:B:99:TYR:CD1	1:B:112:MET:HG2	0.45	2.36	2	2
1:B:133:ALA:HB1	1:B:138:TYR:CB	0.45	2.42	19	1
1:B:51:TYR:CE1	2:B:158:EB4:C3	0.45	3.00	7	1
1:B:84:LYS:O	1:B:102:ARG:NH1	0.45	2.46	10	1
1:B:38:ARG:NH2	1:B:156:GLU:O	0.45	2.46	11	1
1:B:14:TYR:CE2	1:B:119:PRO:HD3	0.45	2.46	18	1
1:B:102:ARG:CD	1:B:109:LEU:HD23	0.45	2.42	3	1
1:B:76:TYR:C	1:B:77:TYR:HD1	0.45	2.20	18	2
1:B:18:LEU:O	1:B:143:VAL:HA	0.45	2.12	18	2
1:B:129:PHE:O	1:B:130:ARG:C	0.45	2.59	12	3
1:B:87:VAL:HA	1:B:98:ILE:CG2	0.45	2.29	20	1
1:B:83:LYS:HZ2	2:B:158:EB4:C14	0.44	2.25	7	2
1:B:53:VAL:HG11	2:B:158:EB4:C21	0.44	2.42	15	1
1:B:15:VAL:HG21	1:B:18:LEU:HD21	0.44	1.90	17	1
1:B:100:ALA:N	1:B:111:MET:O	0.44	2.46	17	1
1:B:47:LEU:CD1	1:B:66:PHE:HB2	0.44	2.42	20	1
1:B:134:GLY:HA2	1:B:138:TYR:HD1	0.44	1.71	1	5
1:B:102:ARG:HD2	2:B:158:EB4:C19	0.44	2.41	1	1
1:B:36:MET:HE1	1:B:153:THR:HG23	0.44	1.89	2	1
1:B:114:LEU:HD21	1:B:125:ALA:CB	0.44	2.38	9	1
1:B:84:LYS:HD3	1:B:86:GLU:OE1	0.44	2.12	11	1
1:B:114:LEU:HD22	1:B:129:PHE:HB2	0.44	1.90	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:83:LYS:HB3	1:B:102:ARG:HG2	0.44	1.88	14	1
1:B:100:ALA:HB2	1:B:113:ARG:HH22	0.44	1.72	15	1
1:B:78:SER:O	1:B:82:LYS:N	0.44	2.51	5	2
1:B:138:TYR:HD2	1:B:143:VAL:HG23	0.44	1.72	13	5
1:B:75:VAL:HG22	1:B:86:GLU:CA	0.44	2.40	6	1
1:B:97:VAL:HG12	1:B:114:LEU:CD1	0.44	2.43	19	1
1:B:112:MET:HE2	1:B:129:PHE:CE2	0.44	2.46	20	1
1:B:64:THR:HG21	2:B:158:EB4:C11	0.44	2.38	9	1
1:B:19:ALA:HA	1:B:142:MET:O	0.44	2.12	15	2
1:B:30:ASP:OD1	1:B:31:LYS:NZ	0.44	2.51	14	3
1:B:21:ASN:OD1	1:B:110:HIS:CD2	0.44	2.71	20	1
1:B:126:THR:CG2	1:B:145:MET:SD	0.44	3.06	20	1
1:B:83:LYS:CE	2:B:158:EB4:C8	0.44	2.92	1	1
1:B:138:TYR:HD2	1:B:143:VAL:CG2	0.44	2.26	17	1
1:B:65:THR:C	1:B:66:PHE:HD1	0.44	2.21	18	1
1:B:62:TRP:CD1	2:B:158:EB4:H14	0.44	2.47	20	1
1:B:114:LEU:C	1:B:114:LEU:CD2	0.44	2.91	20	1
1:B:33:LYS:HB2	1:B:54:PRO:HG3	0.44	1.90	9	1
1:B:60:ARG:HA	1:B:60:ARG:HE	0.44	1.73	15	1
1:B:102:ARG:HG3	2:B:158:EB4:C13	0.44	2.43	17	1
1:B:47:LEU:HD23	1:B:66:PHE:O	0.43	2.12	15	2
1:B:49:VAL:HG11	1:B:66:PHE:CE2	0.43	2.47	13	1
1:B:111:MET:HG3	1:B:113:ARG:NH1	0.43	2.28	14	1
1:B:102:ARG:CG	2:B:158:EB4:C13	0.43	2.95	17	1
1:B:66:PHE:CD1	1:B:78:SER:CB	0.43	2.97	1	2
1:B:15:VAL:HG23	1:B:113:ARG:HG2	0.43	1.90	4	1
1:B:51:TYR:O	1:B:61:LYS:HB2	0.43	2.12	16	1
1:B:102:ARG:HG2	1:B:109:LEU:O	0.43	2.12	20	1
1:B:156:GLU:HG3	1:B:157:VAL:HG12	0.43	1.91	10	1
1:B:48:LYS:HG3	1:B:65:THR:OG1	0.43	2.13	19	1
1:B:27:ARG:O	1:B:31:LYS:HB2	0.43	2.12	20	1
1:B:47:LEU:HD23	1:B:47:LEU:N	0.43	2.28	13	5
1:B:36:MET:N	1:B:52:ALA:O	0.43	2.50	7	3
1:B:32:MET:CA	1:B:32:MET:CE	0.43	2.96	15	1
1:B:32:MET:CA	1:B:32:MET:HE2	0.43	2.42	15	1
1:B:85:VAL:CG1	1:B:100:ALA:HB2	0.43	2.42	18	1
1:B:15:VAL:O	1:B:34:MET:HG2	0.43	2.14	16	1
1:B:47:LEU:HD13	1:B:76:TYR:CZ	0.43	2.47	17	1
1:B:85:VAL:HG12	1:B:100:ALA:HA	0.43	1.90	20	1
1:B:31:LYS:HA	1:B:31:LYS:HZ2	0.43	1.71	3	2
1:B:81:ALA:O	1:B:83:LYS:HE3	0.43	2.14	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:18:LEU:CD2	1:B:113:ARG:CD	0.43	2.95	17	1
1:B:75:VAL:CG1	1:B:86:GLU:HB3	0.43	2.44	20	1
1:B:15:VAL:HG23	1:B:114:LEU:O	0.43	2.13	18	1
1:B:88:LEU:CD1	1:B:99:TYR:HB2	0.43	2.44	5	2
1:B:55:LYS:HD2	1:B:60:ARG:HG3	0.43	1.91	4	1
1:B:47:LEU:CD2	1:B:76:TYR:CD1	0.43	3.01	8	1
1:B:95:TYR:CB	1:B:125:ALA:CB	0.43	2.97	9	1
1:B:138:TYR:CD2	1:B:143:VAL:HG23	0.43	2.48	11	2
1:B:25:PHE:CE1	1:B:111:MET:HE1	0.43	2.49	1	1
1:B:25:PHE:CD2	1:B:111:MET:HE1	0.43	2.48	9	3
1:B:68:LYS:HA	1:B:76:TYR:CD1	0.43	2.49	3	2
1:B:87:VAL:HG23	1:B:98:ILE:HD11	0.43	1.87	20	1
1:B:23:GLU:O	1:B:27:ARG:HB2	0.42	2.14	13	1
1:B:16:VAL:CG2	1:B:114:LEU:HD22	0.42	2.43	17	1
1:B:48:LYS:HG2	1:B:49:VAL:N	0.42	2.28	16	1
1:B:156:GLU:O	1:B:157:VAL:HB	0.42	2.15	8	2
1:B:76:TYR:C	1:B:77:TYR:CD1	0.42	2.98	12	1
1:B:18:LEU:HD22	1:B:29:LYS:HD2	0.42	1.91	16	1
1:B:97:VAL:CB	1:B:112:MET:HE3	0.42	2.41	18	1
1:B:49:VAL:HG21	1:B:66:PHE:CE2	0.42	2.49	13	1
1:B:15:VAL:CG2	1:B:17:ALA:O	0.42	2.64	19	1
1:B:139:THR:OG1	1:B:142:MET:HE3	0.42	2.15	3	1
1:B:35:ALA:HB2	1:B:53:VAL:HG12	0.42	1.92	6	1
1:B:126:THR:CG2	1:B:145:MET:HE3	0.42	2.44	9	1
1:B:46:GLU:OE2	1:B:67:LYS:NZ	0.42	2.50	12	2
1:B:47:LEU:HD22	1:B:76:TYR:CE1	0.42	2.49	12	1
1:B:11:GLY:O	1:B:38:ARG:HG2	0.42	2.14	7	1
1:B:39:ILE:CD1	1:B:49:VAL:HG12	0.42	2.45	15	1
1:B:55:LYS:O	1:B:58:GLY:N	0.42	2.41	15	2
1:B:115:TYR:CD1	1:B:115:TYR:C	0.42	2.97	19	1
1:B:83:LYS:HD2	1:B:102:ARG:HH21	0.42	1.74	1	1
1:B:84:LYS:HE2	1:B:86:GLU:OE2	0.42	2.15	2	1
1:B:33:LYS:O	1:B:34:MET:C	0.42	2.62	15	1
1:B:77:TYR:CD1	1:B:84:LYS:HB3	0.42	2.49	17	1
1:B:51:TYR:O	1:B:61:LYS:CA	0.42	2.66	2	2
1:B:74:GLU:HB3	1:B:87:VAL:HG12	0.42	1.81	19	1
1:B:87:VAL:HG23	1:B:97:VAL:O	0.42	2.15	19	1
1:B:100:ALA:HB3	1:B:113:ARG:HH12	0.42	1.75	5	1
1:B:83:LYS:HZ3	2:B:158:EB4:C11	0.42	2.27	13	1
1:B:18:LEU:O	1:B:144:ALA:N	0.42	2.47	15	1
1:B:114:LEU:HD22	1:B:129:PHE:CB	0.41	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:61:LYS:NZ	1:B:63:GLU:OE2	0.41	2.53	2	2
1:B:77:TYR:CZ	1:B:84:LYS:HG2	0.41	2.50	7	1
1:B:111:MET:SD	1:B:113:ARG:NH2	0.41	2.93	9	1
1:B:126:THR:HG21	1:B:145:MET:HE1	0.41	1.92	15	1
1:B:101:THR:C	1:B:102:ARG:HG3	0.41	2.40	16	1
1:B:16:VAL:CG2	1:B:121:VAL:HG13	0.41	2.44	20	1
1:B:19:ALA:HB1	1:B:143:VAL:HG22	0.41	1.91	20	1
1:B:149:GLN:O	1:B:149:GLN:HG2	0.41	2.14	20	1
1:B:17:ALA:C	1:B:18:LEU:HG	0.41	2.40	1	3
1:B:32:MET:HE2	1:B:32:MET:CA	0.41	2.39	11	1
1:B:111:MET:HB3	1:B:113:ARG:HH11	0.41	1.73	1	1
1:B:126:THR:HG23	1:B:145:MET:HE3	0.41	1.92	9	1
1:B:83:LYS:HB2	1:B:102:ARG:NH2	0.41	2.30	10	1
1:B:46:GLU:HG3	1:B:65:THR:CG2	0.41	2.45	20	1
1:B:77:TYR:OH	1:B:84:LYS:CE	0.41	2.69	5	1
1:B:112:MET:HG2	1:B:129:PHE:CE1	0.41	2.51	17	1
1:B:31:LYS:O	1:B:31:LYS:NZ	0.41	2.49	18	1
1:B:47:LEU:HD21	1:B:66:PHE:HB2	0.41	1.93	15	2
1:B:126:THR:CG2	1:B:145:MET:CE	0.41	2.98	15	1
1:B:3:VAL:HB	1:B:4:PRO:HD2	0.41	1.93	18	1
1:B:49:VAL:CG2	1:B:66:PHE:HE1	0.41	2.29	2	1
1:B:42:LEU:CG	1:B:46:GLU:HG2	0.41	2.46	8	1
1:B:25:PHE:O	1:B:29:LYS:N	0.41	2.50	13	1
1:B:78:SER:OG	1:B:83:LYS:HB2	0.41	2.15	15	1
1:B:114:LEU:HD12	1:B:129:PHE:CG	0.41	2.50	17	1
1:B:19:ALA:HB3	1:B:112:MET:N	0.41	2.30	20	1
1:B:84:LYS:HG2	1:B:101:THR:O	0.41	2.16	8	1
1:B:25:PHE:CE2	2:B:158:EB4:C19	0.41	3.04	12	1
2:B:158:EB4:O2	2:B:158:EB4:N2	0.41	2.54	16	3
1:B:47:LEU:O	1:B:66:PHE:N	0.41	2.51	6	1
1:B:148:ARG:HD2	1:B:148:ARG:N	0.41	2.29	16	3
1:B:91:ASP:HB3	1:B:94:SER:CB	0.41	2.35	12	1
1:B:77:TYR:CE2	1:B:84:LYS:HG3	0.41	2.51	13	1
1:B:84:LYS:NZ	1:B:86:GLU:OE1	0.41	2.54	15	1
1:B:82:LYS:CA	1:B:103:VAL:HG12	0.41	2.46	17	1
1:B:19:ALA:CB	1:B:112:MET:O	0.41	2.68	18	1
1:B:95:TYR:CZ	1:B:125:ALA:CA	0.41	3.02	18	1
1:B:84:LYS:NZ	1:B:86:GLU:OE2	0.41	2.52	20	1
1:B:62:TRP:CD1	2:B:158:EB4:O8	0.41	2.73	18	1
1:B:14:TYR:CD2	1:B:119:PRO:HB3	0.40	2.50	6	1
1:B:51:TYR:CE2	2:B:158:EB4:C8	0.40	3.04	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:THR:O	1:B:75:VAL:C	0.40	2.63	20	1
1:B:25:PHE:O	1:B:29:LYS:NZ	0.40	2.51	15	1
1:B:40:SER:N	1:B:48:LYS:O	0.40	2.38	16	1
1:B:90:THR:OG1	1:B:96:ALA:CB	0.40	2.70	18	1
1:B:110:HIS:O	1:B:111:MET:HG3	0.40	2.16	18	1
1:B:47:LEU:HD11	1:B:66:PHE:HB2	0.40	1.91	20	1
1:B:146:LEU:N	1:B:146:LEU:HD22	0.40	2.31	20	1
1:B:133:ALA:C	1:B:138:TYR:CD1	0.40	3.00	14	1
1:B:15:VAL:HG21	1:B:18:LEU:CD2	0.40	2.47	17	1
1:B:69:THR:CB	1:B:77:TYR:CD1	0.40	3.04	1	1
1:B:25:PHE:CE2	1:B:111:MET:CE	0.40	3.04	13	1
1:B:143:VAL:HG12	1:B:144:ALA:N	0.40	2.32	13	1
1:B:72:ASP:OD1	1:B:72:ASP:C	0.40	2.63	14	1
1:B:104:LYS:HG2	1:B:105:ASP:H	0.40	1.76	18	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	B	155/157 (99%)	138±2 (89±1%)	13±2 (8±1%)	4±1 (2±1%)	7	45
All	All	3100/3140 (99%)	2769 (89%)	260 (8%)	71 (2%)	7	45

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	148	ARG	19
1	B	105	ASP	18
1	B	151	GLU	15
1	B	147	PRO	7
1	B	32	MET	6
1	B	33	LYS	3
1	B	56	PRO	1
1	B	73	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	B	57	ASN	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	B	137/137 (100%)	119±3 (87±2%)	18±3 (13±2%)	6	46
All	All	2740/2740 (100%)	2379 (87%)	361 (13%)	6	46

All 64 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	B	31	LYS	20
1	B	29	LYS	19
1	B	153	THR	17
1	B	148	ARG	15
1	B	7	SER	15
1	B	21	ASN	14
1	B	22	THR	14
1	B	63	GLU	13
1	B	102	ARG	11
1	B	113	ARG	11
1	B	78	SER	11
1	B	23	GLU	10
1	B	70	SER	10
1	B	42	LEU	9
1	B	139	THR	9
1	B	79	GLU	9
1	B	60	ARG	9
1	B	86	GLU	8
1	B	65	THR	8
1	B	108	THR	7
1	B	6	ARG	7
1	B	69	THR	6
1	B	61	LYS	6
1	B	84	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	B	64	THR	6
1	B	150	GLU	6
1	B	32	MET	6
1	B	51	TYR	5
1	B	149	GLN	5
1	B	30	ASP	5
1	B	140	ASP	4
1	B	138	TYR	4
1	B	83	LYS	3
1	B	101	THR	3
1	B	104	LYS	3
1	B	122	SER	3
1	B	82	LYS	3
1	B	72	ASP	2
1	B	107	ARG	2
1	B	117	ARG	2
1	B	155	ASP	2
1	B	136	ARG	2
1	B	74	GLU	2
1	B	5	ASP	2
1	B	28	GLU	2
1	B	105	ASP	2
1	B	67	LYS	2
1	B	130	ARG	2
1	B	47	LEU	2
1	B	50	SER	2
1	B	121	VAL	2
1	B	135	GLU	1
1	B	12	LYS	1
1	B	36	MET	1
1	B	27	ARG	1
1	B	15	VAL	1
1	B	38	ARG	1
1	B	141	GLU	1
1	B	109	LEU	1
1	B	62	TRP	1
1	B	115	TYR	1
1	B	13	TRP	1
1	B	44	GLU	1
1	B	120	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	EB4	B	158	3	51,51,51	1.03±0.02	1±0 (1±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	EB4	B	158	3	72,72,72	1.18±0.02	10±1 (13±1%)

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	EB4	B	158	3	-	0±0,51,51,51	0±0,3,4,4

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	158	EB4	C17-C20	5.87	1.38	1.50	11	20

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
2	B	158	EB4	O1-C1-C16	3.53	127.41	121.11	2	20
2	B	158	EB4	O3-C3-C18	3.04	126.53	121.11	4	20
2	B	158	EB4	O2-C2-C17	3.03	126.52	121.11	4	20
2	B	158	EB4	O4-C4-C7	3.02	127.45	119.36	5	20
2	B	158	EB4	O5-C5-C8	2.78	126.82	119.36	8	20
2	B	158	EB4	O1-C1-C4	2.65	112.48	119.46	1	20
2	B	158	EB4	O6-C6-C9	2.59	126.31	119.36	5	20
2	B	158	EB4	O3-C3-C6	2.42	113.08	119.46	8	18
2	B	158	EB4	C28-C22-C25	2.30	115.68	109.88	3	9
2	B	158	EB4	O2-C2-C5	2.29	113.44	119.46	4	16
2	B	158	EB4	C29-O14-C27	2.27	111.32	116.78	9	1
2	B	158	EB4	O4-C4-C1	2.16	112.34	117.90	18	4
2	B	158	EB4	O14-C27-C24	2.03	116.35	111.58	12	1
2	B	158	EB4	O15-C25-C22	2.02	116.34	111.58	20	1

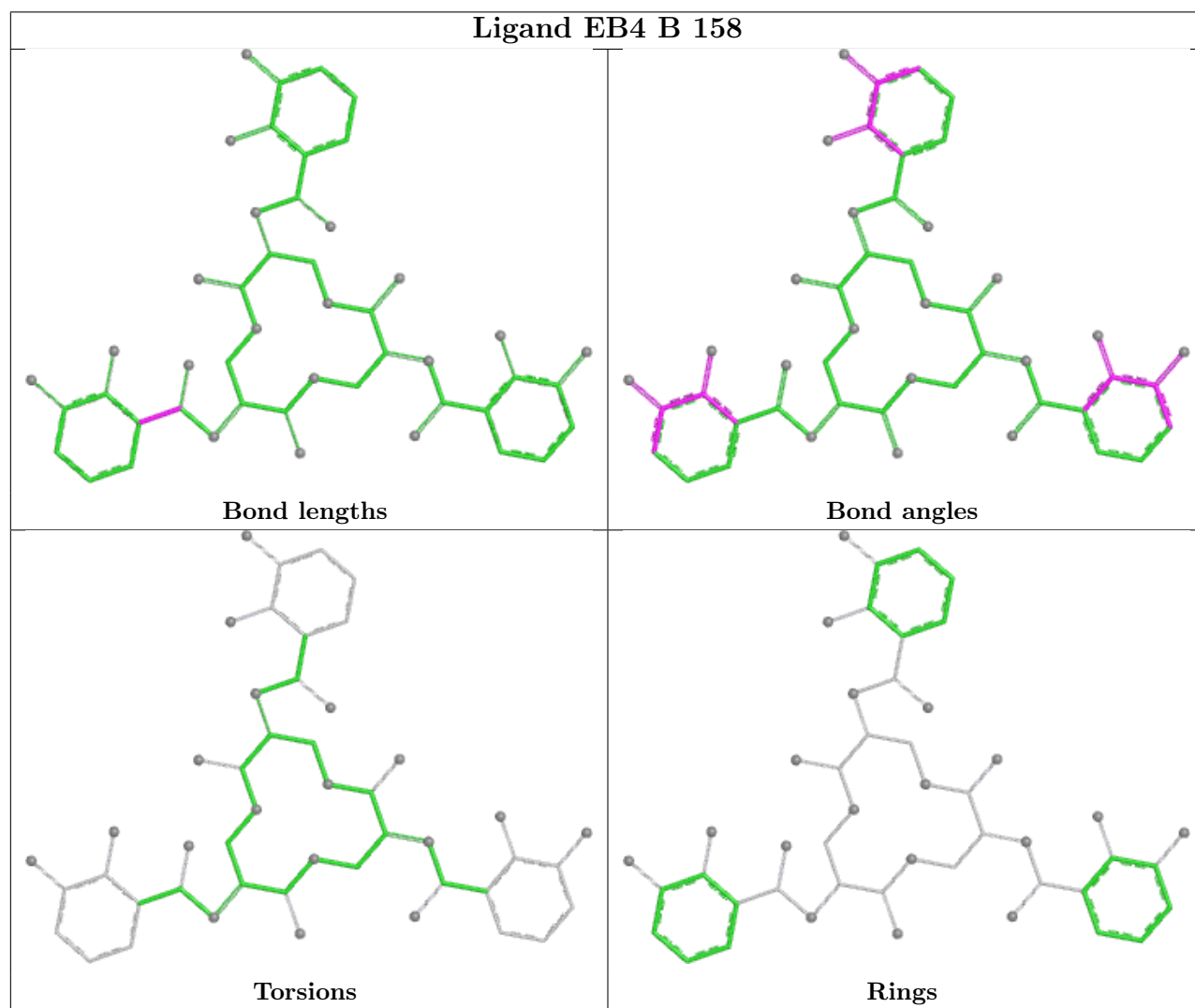
There are no chirality outliers.

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