



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 PM UTC

PDB ID : 1HJ7 / pdb_00001hj7
Title : NMR study of a pair of LDL receptor Ca²⁺ binding epidermal growth factor-like domains, 20 structures
Authors : Saha, S.; Handford, P.A.; Campbell, I.D.; Downing, A.K.
Deposited on : 2001-01-09

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

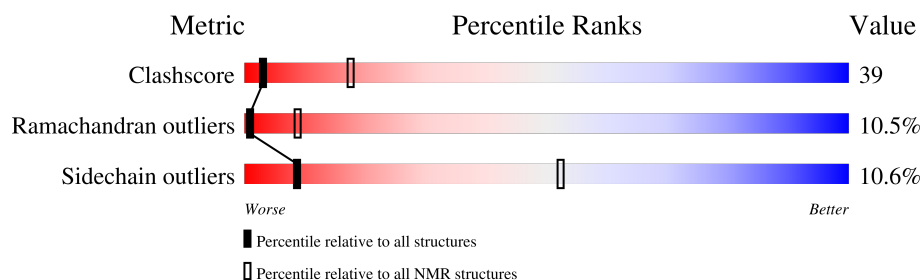
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

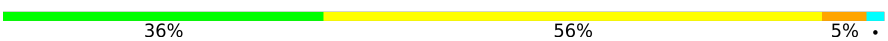
The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	80	

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.

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:295-A:372 (78)	1.32	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 5 clusters. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1151 atoms, of which 542 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LDL RECEPTOR.

Mol	Chain	Residues	Atoms						Trace
1	A	80	Total	C	H	N	O	S	0
			1149	361	542	105	129	12	

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

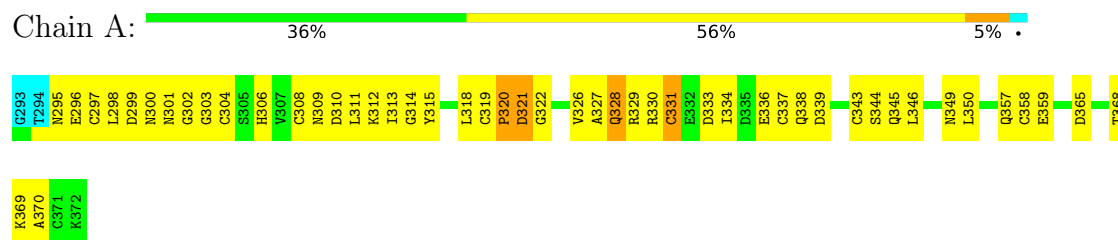
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

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: LDL RECEPTOR

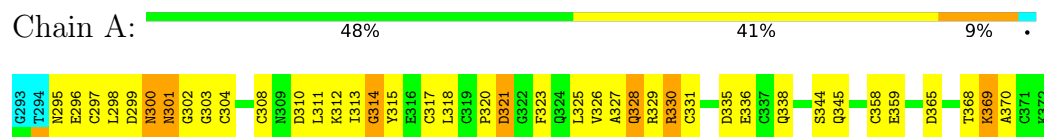


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

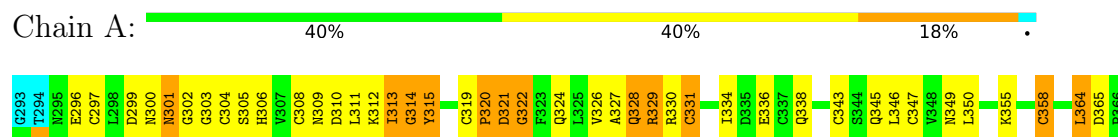
4.2.1 Score per residue for model 1

• Molecule 1: LDL RECEPTOR



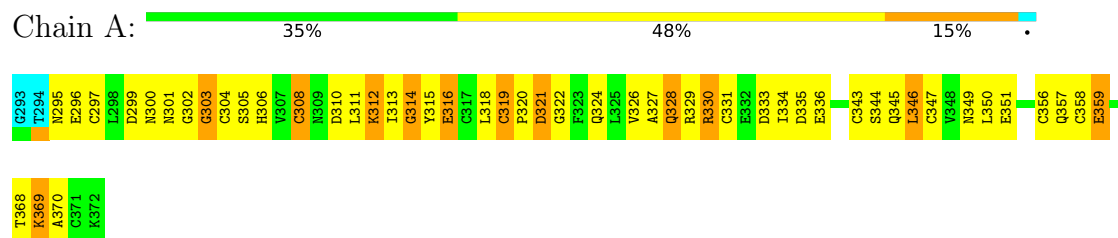
4.2.2 Score per residue for model 2

• Molecule 1: LDL RECEPTOR



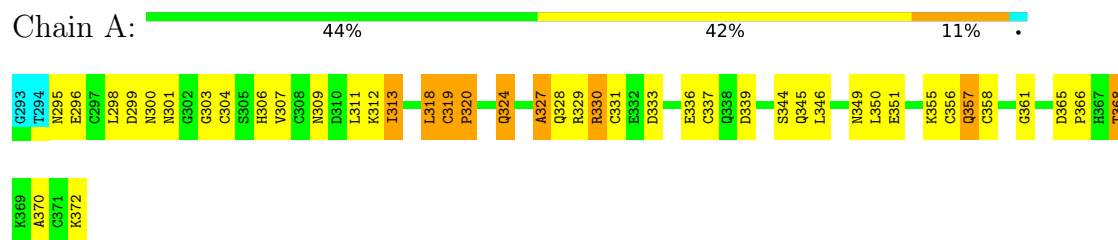
4.2.3 Score per residue for model 3

- Molecule 1: LDL RECEPTOR



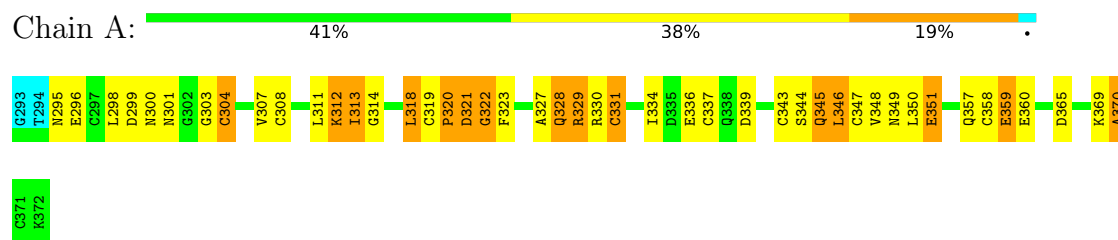
4.2.4 Score per residue for model 4

- Molecule 1: LDL RECEPTOR



4.2.5 Score per residue for model 5

- Molecule 1: LDL RECEPTOR



4.2.6 Score per residue for model 6

- Molecule 1: LDL RECEPTOR

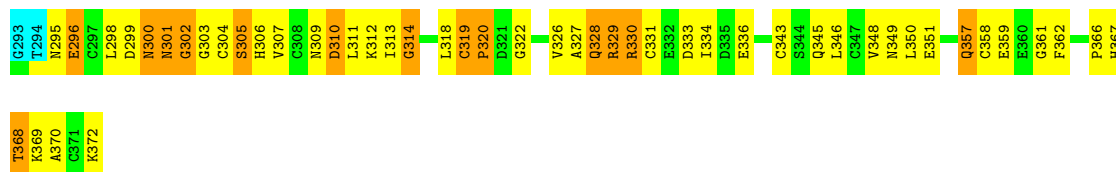




4.2.7 Score per residue for model 7

- Molecule 1: LDL RECEPTOR

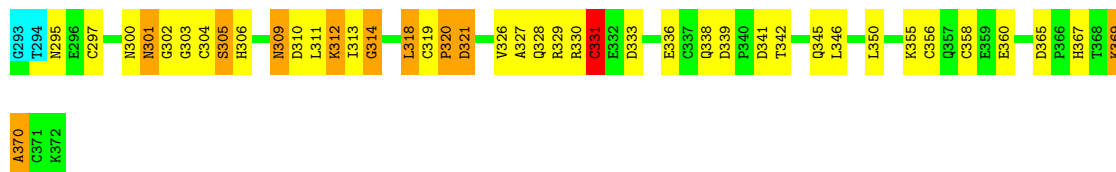
Chain A: 36% 44% 18%



4.2.8 Score per residue for model 8

- Molecule 1: LDL RECEPTOR

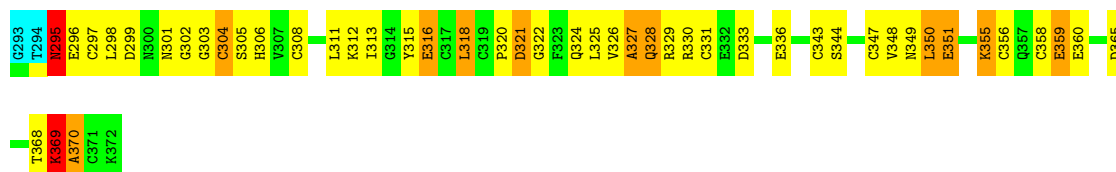
Chain A: 45% 39% 12%



4.2.9 Score per residue for model 9

- Molecule 1: LDL RECEPTOR

Chain A: 39% 42% 14%



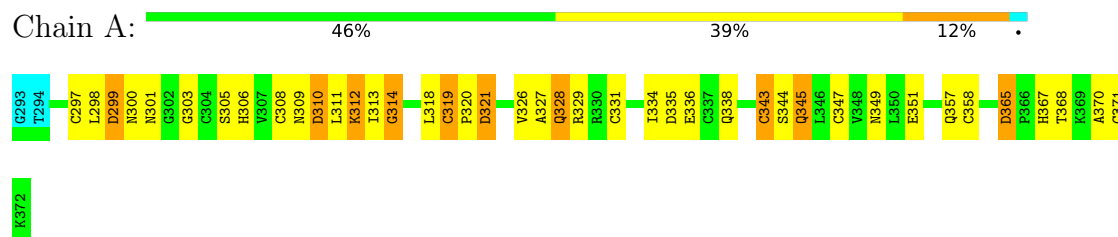
4.2.10 Score per residue for model 10

- Molecule 1: LDL RECEPTOR



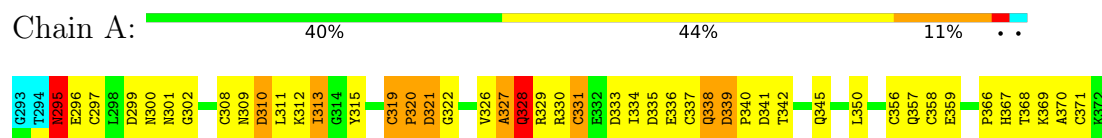
4.2.11 Score per residue for model 11

- Molecule 1: LDL RECEPTOR



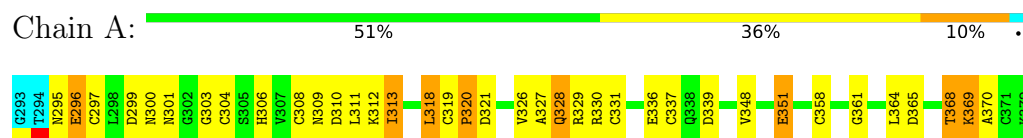
4.2.12 Score per residue for model 12

- Molecule 1: LDL RECEPTOR



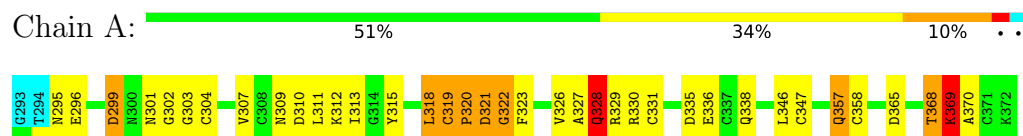
4.2.13 Score per residue for model 13

- Molecule 1: LDL RECEPTOR



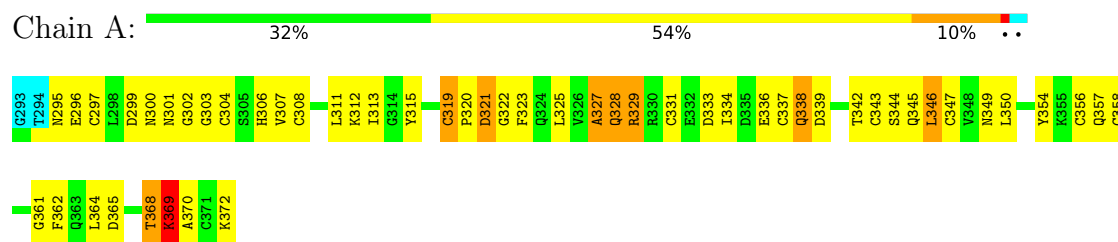
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: LDL RECEPTOR



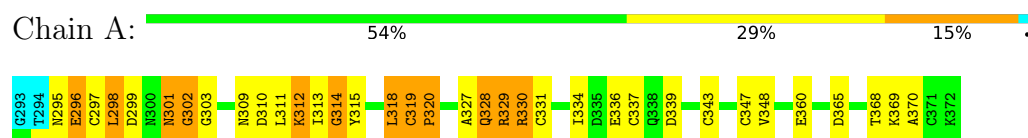
4.2.15 Score per residue for model 15

- Molecule 1: LDL RECEPTOR



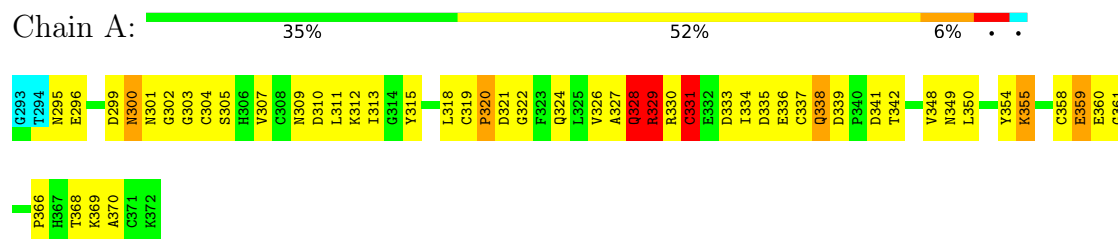
4.2.16 Score per residue for model 16

- Molecule 1: LDL RECEPTOR



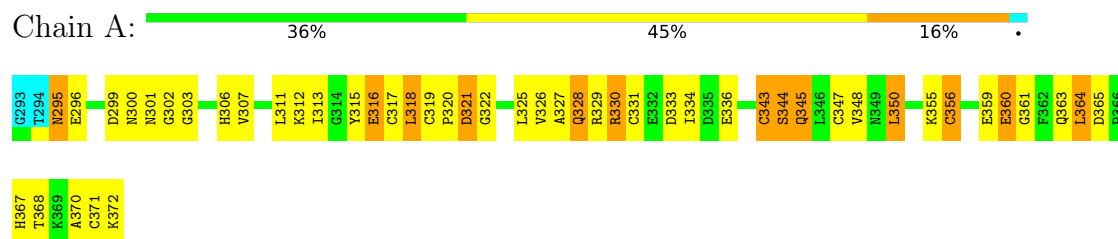
4.2.17 Score per residue for model 17

- Molecule 1: LDL RECEPTOR



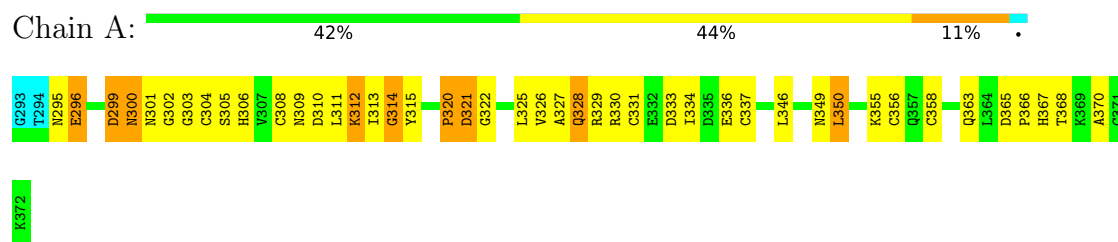
4.2.18 Score per residue for model 18

- Molecule 1: LDL RECEPTOR



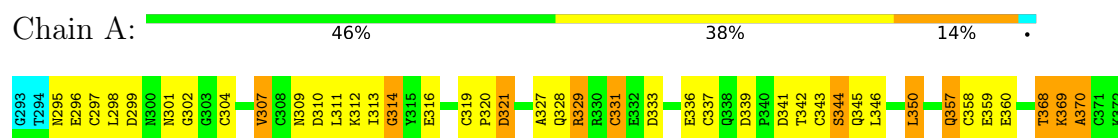
4.2.19 Score per residue for model 19

- Molecule 1: LDL RECEPTOR



4.2.20 Score per residue for model 20

- Molecule 1: LDL RECEPTOR



5 Refinement protocol and experimental data overview

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

Of the 280 calculated structures, 20 were deposited, based on the following criterion: *NO NOE, 3JHN OR 1JHN CONSTRAINTS VIOLATED BY > 0.5 Å, 5 DEGREES OR 2 HERTZ*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
X-PLOR	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:
CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.50±0.02	0±0/604 (0.0± 0.1%)	1.22±0.03	1±1/812 (0.1± 0.1%)
All	All	1.50	6/12080 (0.0%)	1.22	17/16240 (0.1%)

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	A	350	LEU	N-CA	6.63	1.50	1.46	9	4
1	A	299	ASP	N-CA	6.22	1.50	1.46	14	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	322	GLY	N-CA-C	-6.15	107.29	115.40	2	2
1	A	299	ASP	CA-C-O	5.70	121.24	117.94	14	2
1	A	350	LEU	CB-CA-C	-5.65	108.93	117.07	9	5
1	A	302	GLY	N-CA-C	-5.46	108.48	115.42	16	1
1	A	299	ASP	CB-CA-C	-5.36	109.35	117.07	11	2
1	A	329	ARG	N-CA-C	-5.33	108.54	114.62	17	1
1	A	350	LEU	CA-C-O	5.29	121.01	117.94	2	4

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	596	532	530	44±6
All	All	11960	10640	10600	871

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:PRO:O	1:A:322:GLY:N	0.87	2.07	19	4
1:A:326:VAL:HG13	1:A:327:ALA:H	0.76	1.40	17	3
1:A:298:LEU:HD22	1:A:298:LEU:N	0.67	2.04	20	6
1:A:297:CYS:O	1:A:299:ASP:N	0.67	2.27	16	2
1:A:343:CYS:SG	1:A:344:SER:N	0.66	2.68	3	4
1:A:326:VAL:HG13	1:A:327:ALA:N	0.65	2.06	11	3
1:A:368:THR:OG1	1:A:369:LYS:N	0.65	2.29	15	6
1:A:296:GLU:H	1:A:296:GLU:CD	0.64	2.01	7	1
1:A:327:ALA:O	1:A:329:ARG:N	0.62	2.33	8	11
1:A:321:ASP:O	1:A:323:PHE:N	0.62	2.33	14	4
1:A:320:PRO:O	1:A:321:ASP:O	0.62	2.18	8	3
1:A:320:PRO:O	1:A:321:ASP:C	0.60	2.45	18	7
1:A:301:ASN:ND2	1:A:308:CYS:SG	0.60	2.74	19	2
1:A:311:LEU:O	1:A:313:ILE:N	0.60	2.34	12	4
1:A:306:HIS:ND1	1:A:319:CYS:SG	0.60	2.75	7	3
1:A:319:CYS:O	1:A:320:PRO:O	0.60	2.19	17	5
1:A:345:GLN:NE2	1:A:356:CYS:SG	0.59	2.75	18	1
1:A:309:ASN:HD22	1:A:311:LEU:HD21	0.59	1.57	14	2
1:A:319:CYS:O	1:A:321:ASP:N	0.59	2.36	2	4
1:A:320:PRO:O	1:A:321:ASP:CB	0.58	2.52	1	8
1:A:336:GLU:N	1:A:349:ASN:HD21	0.58	1.96	19	2
1:A:336:GLU:H	1:A:336:GLU:CD	0.57	2.08	13	17
1:A:300:ASN:O	1:A:302:GLY:N	0.57	2.38	7	1
1:A:327:ALA:O	1:A:328:GLN:CB	0.57	2.52	10	9
1:A:336:GLU:H	1:A:349:ASN:HD21	0.56	1.43	19	2
1:A:322:GLY:O	1:A:334:ILE:HG22	0.56	2.00	10	8
1:A:342:THR:CG2	1:A:354:TYR:CE2	0.56	2.88	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:295:ASN:HB2	1:A:298:LEU:HD22	0.56	1.78	5	1
1:A:351:GLU:H	1:A:351:GLU:CD	0.56	2.07	13	1
1:A:306:HIS:CG	1:A:319:CYS:SG	0.56	2.98	6	3
1:A:298:LEU:N	1:A:298:LEU:CD2	0.56	2.68	11	6
1:A:360:GLU:H	1:A:360:GLU:CD	0.56	2.09	18	2
1:A:369:LYS:CD	1:A:369:LYS:N	0.55	2.70	9	1
1:A:304:CYS:O	1:A:306:HIS:N	0.55	2.40	8	4
1:A:326:VAL:O	1:A:328:GLN:N	0.55	2.39	7	2
1:A:303:GLY:O	1:A:329:ARG:NH1	0.55	2.40	18	5
1:A:298:LEU:H	1:A:298:LEU:CD2	0.55	2.14	16	1
1:A:347:CYS:SG	1:A:347:CYS:O	0.55	2.64	3	5
1:A:304:CYS:SG	1:A:305:SER:N	0.55	2.80	9	1
1:A:365:ASP:OD1	1:A:369:LYS:N	0.55	2.39	10	1
1:A:298:LEU:N	1:A:298:LEU:CD1	0.54	2.70	5	1
1:A:348:VAL:CG1	1:A:350:LEU:HD21	0.54	2.32	7	1
1:A:297:CYS:O	1:A:301:ASN:N	0.54	2.40	16	2
1:A:301:ASN:ND2	1:A:304:CYS:O	0.54	2.41	8	7
1:A:301:ASN:ND2	1:A:304:CYS:N	0.54	2.55	17	1
1:A:296:GLU:N	1:A:296:GLU:OE1	0.54	2.40	6	9
1:A:345:GLN:HE22	1:A:364:LEU:HD21	0.54	1.63	18	1
1:A:315:TYR:HH	1:A:329:ARG:NH1	0.54	2.00	1	1
1:A:302:GLY:C	1:A:304:CYS:H	0.54	2.11	1	6
1:A:299:ASP:O	1:A:301:ASN:N	0.54	2.41	6	5
1:A:336:GLU:OE1	1:A:349:ASN:ND2	0.54	2.41	7	3
1:A:300:ASN:O	1:A:301:ASN:C	0.54	2.50	7	1
1:A:302:GLY:O	1:A:304:CYS:N	0.54	2.41	8	6
1:A:301:ASN:O	1:A:301:ASN:ND2	0.54	2.41	3	4
1:A:329:ARG:HH11	1:A:329:ARG:CG	0.54	2.16	11	3
1:A:316:GLU:OE2	1:A:318:LEU:N	0.53	2.41	18	3
1:A:365:ASP:OD2	1:A:370:ALA:N	0.53	2.40	10	1
1:A:335:ASP:OD1	1:A:338:GLN:N	0.53	2.42	1	3
1:A:343:CYS:SG	1:A:346:LEU:O	0.53	2.67	3	4
1:A:344:SER:O	1:A:345:GLN:CB	0.53	2.55	18	3
1:A:346:LEU:N	1:A:346:LEU:HD22	0.53	2.18	14	4
1:A:329:ARG:CG	1:A:329:ARG:NH1	0.53	2.71	11	3
1:A:301:ASN:ND2	1:A:301:ASN:O	0.53	2.41	2	3
1:A:297:CYS:O	1:A:298:LEU:C	0.53	2.51	16	2
1:A:337:CYS:O	1:A:339:ASP:N	0.53	2.41	15	5
1:A:346:LEU:N	1:A:346:LEU:CD2	0.53	2.71	14	5
1:A:365:ASP:CG	1:A:369:LYS:N	0.53	2.66	15	2
1:A:336:GLU:N	1:A:336:GLU:OE2	0.53	2.42	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:315:TYR:OH	1:A:329:ARG:NH1	0.53	2.42	12	2
1:A:330:ARG:NH1	1:A:330:ARG:CG	0.53	2.72	4	4
1:A:297:CYS:SG	1:A:308:CYS:C	0.53	2.92	3	3
1:A:355:LYS:O	1:A:357:GLN:NE2	0.53	2.42	4	1
1:A:301:ASN:HD22	1:A:304:CYS:N	0.53	2.02	7	1
1:A:337:CYS:C	1:A:339:ASP:N	0.52	2.67	6	10
1:A:296:GLU:CD	1:A:296:GLU:N	0.52	2.67	7	2
1:A:365:ASP:OD2	1:A:367:HIS:NE2	0.52	2.42	8	1
1:A:368:THR:O	1:A:370:ALA:N	0.52	2.41	1	7
1:A:329:ARG:NH1	1:A:329:ARG:CG	0.52	2.72	20	3
1:A:338:GLN:N	1:A:338:GLN:OE1	0.52	2.41	17	1
1:A:330:ARG:O	1:A:331:CYS:SG	0.52	2.68	17	10
1:A:299:ASP:C	1:A:301:ASN:N	0.52	2.67	12	7
1:A:302:GLY:C	1:A:304:CYS:N	0.52	2.67	14	6
1:A:320:PRO:O	1:A:321:ASP:CG	0.52	2.53	11	4
1:A:301:ASN:O	1:A:303:GLY:N	0.52	2.42	7	1
1:A:357:GLN:HE22	1:A:362:PHE:H	0.52	1.45	7	1
1:A:327:ALA:O	1:A:328:GLN:NE2	0.52	2.42	13	1
1:A:338:GLN:OE1	1:A:338:GLN:CA	0.52	2.57	17	1
1:A:341:ASP:OD1	1:A:342:THR:N	0.52	2.42	20	1
1:A:359:GLU:CD	1:A:360:GLU:N	0.52	2.67	5	1
1:A:310:ASP:OD1	1:A:311:LEU:N	0.52	2.42	16	1
1:A:295:ASN:N	1:A:295:ASN:OD1	0.52	2.43	1	7
1:A:351:GLU:N	1:A:351:GLU:CD	0.52	2.67	3	1
1:A:363:GLN:CD	1:A:364:LEU:N	0.52	2.68	18	1
1:A:327:ALA:C	1:A:329:ARG:N	0.52	2.68	8	11
1:A:351:GLU:CD	1:A:351:GLU:N	0.52	2.67	13	1
1:A:351:GLU:N	1:A:351:GLU:OE1	0.52	2.43	3	2
1:A:365:ASP:OD2	1:A:369:LYS:N	0.52	2.43	15	1
1:A:368:THR:C	1:A:370:ALA:N	0.51	2.68	12	8
1:A:343:CYS:O	1:A:345:GLN:N	0.51	2.43	18	1
1:A:305:SER:O	1:A:306:HIS:CD2	0.51	2.63	9	2
1:A:314:GLY:O	1:A:315:TYR:O	0.51	2.29	6	1
1:A:344:SER:O	1:A:345:GLN:CG	0.51	2.59	18	1
1:A:343:CYS:SG	1:A:357:GLN:N	0.51	2.83	10	2
1:A:337:CYS:H	1:A:349:ASN:HD22	0.51	1.47	19	1
1:A:363:GLN:N	1:A:363:GLN:CD	0.51	2.68	19	1
1:A:329:ARG:CG	1:A:329:ARG:HH11	0.51	2.18	2	3
1:A:297:CYS:SG	1:A:308:CYS:O	0.51	2.69	11	6
1:A:304:CYS:SG	1:A:329:ARG:O	0.51	2.69	5	1
1:A:321:ASP:C	1:A:323:PHE:H	0.51	2.12	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:357:GLN:O	1:A:358:CYS:SG	0.51	2.69	11	1
1:A:355:LYS:C	1:A:356:CYS:SG	0.51	2.94	9	2
1:A:295:ASN:CB	1:A:298:LEU:HD22	0.51	2.36	5	1
1:A:365:ASP:CG	1:A:370:ALA:N	0.51	2.69	10	1
1:A:300:ASN:O	1:A:301:ASN:CB	0.51	2.58	13	2
1:A:326:VAL:CG1	1:A:327:ALA:H	0.51	2.18	11	3
1:A:295:ASN:ND2	1:A:299:ASP:OD1	0.51	2.44	20	2
1:A:330:ARG:CG	1:A:330:ARG:HH11	0.51	2.18	7	3
1:A:326:VAL:O	1:A:327:ALA:HB3	0.51	2.06	2	1
1:A:327:ALA:O	1:A:328:GLN:CG	0.51	2.59	2	5
1:A:330:ARG:CG	1:A:331:CYS:H	0.51	2.19	9	3
1:A:368:THR:O	1:A:369:LYS:CB	0.51	2.59	13	1
1:A:304:CYS:C	1:A:306:HIS:N	0.50	2.67	8	5
1:A:335:ASP:CG	1:A:349:ASN:ND2	0.50	2.69	17	1
1:A:363:GLN:N	1:A:372:LYS:O	0.50	2.44	6	1
1:A:337:CYS:SG	1:A:337:CYS:O	0.50	2.70	16	1
1:A:335:ASP:CG	1:A:349:ASN:HD22	0.50	2.14	17	1
1:A:320:PRO:C	1:A:322:GLY:N	0.50	2.68	19	1
1:A:371:CYS:SG	1:A:371:CYS:O	0.50	2.69	2	2
1:A:300:ASN:O	1:A:300:ASN:ND2	0.50	2.44	3	1
1:A:295:ASN:O	1:A:295:ASN:ND2	0.50	2.44	14	1
1:A:337:CYS:H	1:A:349:ASN:ND2	0.50	2.05	19	1
1:A:357:GLN:C	1:A:358:CYS:SG	0.50	2.95	14	3
1:A:365:ASP:OD1	1:A:372:LYS:NZ	0.50	2.42	18	1
1:A:318:LEU:C	1:A:319:CYS:SG	0.50	2.94	4	4
1:A:357:GLN:HE22	1:A:362:PHE:N	0.50	2.05	7	1
1:A:345:GLN:NE2	1:A:359:GLU:OE1	0.49	2.45	3	1
1:A:301:ASN:OD1	1:A:308:CYS:SG	0.49	2.70	6	1
1:A:324:GLN:NE2	1:A:333:ASP:O	0.49	2.45	6	2
1:A:304:CYS:SG	1:A:307:VAL:O	0.49	2.70	14	3
1:A:295:ASN:C	1:A:297:CYS:H	0.49	2.14	16	2
1:A:345:GLN:CD	1:A:356:CYS:SG	0.49	2.94	18	1
1:A:300:ASN:C	1:A:302:GLY:H	0.49	2.15	10	3
1:A:345:GLN:CD	1:A:358:CYS:SG	0.49	2.95	11	2
1:A:339:ASP:N	1:A:339:ASP:OD1	0.49	2.43	12	3
1:A:367:HIS:ND1	1:A:368:THR:N	0.49	2.61	18	2
1:A:326:VAL:O	1:A:326:VAL:HG22	0.49	2.08	12	2
1:A:326:VAL:CG1	1:A:330:ARG:O	0.49	2.61	6	1
1:A:365:ASP:OD2	1:A:367:HIS:CD2	0.49	2.66	8	1
1:A:299:ASP:C	1:A:301:ASN:H	0.49	2.16	2	12
1:A:296:GLU:N	1:A:296:GLU:OE2	0.49	2.45	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:345:GLN:NE2	1:A:371:CYS:SG	0.49	2.85	12	1
1:A:296:GLU:CB	1:A:315:TYR:CD2	0.49	2.95	19	1
1:A:365:ASP:OD2	1:A:372:LYS:NZ	0.49	2.42	4	1
1:A:318:LEU:O	1:A:319:CYS:SG	0.49	2.70	6	3
1:A:360:GLU:N	1:A:360:GLU:OE2	0.49	2.45	16	1
1:A:311:LEU:O	1:A:312:LYS:C	0.49	2.56	17	13
1:A:327:ALA:C	1:A:329:ARG:H	0.49	2.15	4	4
1:A:359:GLU:CD	1:A:360:GLU:H	0.49	2.16	5	1
1:A:326:VAL:CG1	1:A:327:ALA:N	0.49	2.75	11	4
1:A:295:ASN:N	1:A:310:ASP:OD2	0.49	2.46	3	1
1:A:301:ASN:C	1:A:303:GLY:N	0.49	2.68	7	2
1:A:299:ASP:C	1:A:300:ASN:ND2	0.49	2.71	15	1
1:A:363:GLN:N	1:A:363:GLN:OE1	0.49	2.46	19	1
1:A:309:ASN:HD22	1:A:309:ASN:C	0.49	2.15	8	2
1:A:359:GLU:O	1:A:361:GLY:N	0.49	2.45	18	1
1:A:364:LEU:HD13	1:A:365:ASP:N	0.48	2.22	18	2
1:A:307:VAL:HG12	1:A:308:CYS:N	0.48	2.23	15	2
1:A:313:ILE:O	1:A:314:GLY:O	0.48	2.31	11	10
1:A:301:ASN:C	1:A:303:GLY:H	0.48	2.16	4	7
1:A:321:ASP:C	1:A:323:PHE:N	0.48	2.70	14	2
1:A:307:VAL:CG1	1:A:308:CYS:N	0.48	2.76	15	2
1:A:295:ASN:O	1:A:297:CYS:N	0.48	2.46	16	1
1:A:355:LYS:O	1:A:356:CYS:SG	0.48	2.72	9	3
1:A:327:ALA:O	1:A:328:GLN:C	0.48	2.56	9	8
1:A:368:THR:C	1:A:370:ALA:H	0.48	2.15	12	8
1:A:344:SER:O	1:A:358:CYS:SG	0.48	2.72	10	2
1:A:346:LEU:HD23	1:A:347:CYS:N	0.48	2.24	3	1
1:A:365:ASP:CB	1:A:368:THR:OG1	0.48	2.62	4	2
1:A:328:GLN:O	1:A:328:GLN:CG	0.48	2.61	3	2
1:A:300:ASN:C	1:A:302:GLY:N	0.47	2.71	19	3
1:A:300:ASN:O	1:A:301:ASN:CG	0.47	2.57	5	2
1:A:365:ASP:CG	1:A:369:LYS:CA	0.47	2.87	15	2
1:A:302:GLY:CA	1:A:315:TYR:OH	0.47	2.62	2	6
1:A:309:ASN:O	1:A:310:ASP:C	0.47	2.56	7	7
1:A:326:VAL:O	1:A:327:ALA:C	0.47	2.56	9	1
1:A:297:CYS:C	1:A:299:ASP:N	0.47	2.72	16	2
1:A:319:CYS:C	1:A:321:ASP:N	0.47	2.72	12	2
1:A:321:ASP:C	1:A:321:ASP:OD1	0.47	2.57	11	1
1:A:308:CYS:O	1:A:308:CYS:SG	0.47	2.72	13	3
1:A:345:GLN:HE22	1:A:359:GLU:CD	0.47	2.18	3	1
1:A:328:GLN:CG	1:A:328:GLN:O	0.47	2.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:358:CYS:O	1:A:359:GLU:O	0.47	2.33	9	1
1:A:296:GLU:N	1:A:296:GLU:CD	0.47	2.73	12	1
1:A:359:GLU:CD	1:A:359:GLU:N	0.47	2.73	1	1
1:A:299:ASP:C	1:A:300:ASN:HD22	0.47	2.18	15	1
1:A:336:GLU:CD	1:A:336:GLU:N	0.47	2.73	5	12
1:A:337:CYS:C	1:A:339:ASP:H	0.47	2.18	10	5
1:A:297:CYS:C	1:A:298:LEU:HD22	0.46	2.34	20	2
1:A:364:LEU:C	1:A:364:LEU:HD13	0.46	2.34	2	1
1:A:345:GLN:OE1	1:A:358:CYS:SG	0.46	2.73	1	2
1:A:295:ASN:O	1:A:295:ASN:CG	0.46	2.57	17	6
1:A:330:ARG:CG	1:A:331:CYS:N	0.46	2.78	14	3
1:A:346:LEU:N	1:A:346:LEU:HD12	0.46	2.25	8	1
1:A:335:ASP:CG	1:A:338:GLN:OE1	0.46	2.58	17	1
1:A:317:CYS:O	1:A:325:LEU:HD13	0.46	2.10	18	2
1:A:330:ARG:CD	1:A:331:CYS:H	0.46	2.23	8	1
1:A:320:PRO:O	1:A:321:ASP:OD2	0.46	2.34	11	1
1:A:348:VAL:O	1:A:348:VAL:CG1	0.46	2.64	18	3
1:A:348:VAL:O	1:A:348:VAL:HG13	0.46	2.09	18	3
1:A:345:GLN:CG	1:A:356:CYS:SG	0.46	3.03	18	1
1:A:365:ASP:CG	1:A:370:ALA:H	0.46	2.19	10	1
1:A:298:LEU:N	1:A:298:LEU:HD12	0.46	2.26	5	1
1:A:300:ASN:O	1:A:301:ASN:OD1	0.46	2.33	8	2
1:A:365:ASP:OD1	1:A:367:HIS:CD2	0.46	2.69	8	1
1:A:302:GLY:O	1:A:315:TYR:OH	0.46	2.34	12	6
1:A:364:LEU:HD11	1:A:369:LYS:O	0.46	2.10	13	1
1:A:326:VAL:HG23	1:A:327:ALA:N	0.46	2.25	19	1
1:A:300:ASN:ND2	1:A:300:ASN:N	0.45	2.63	1	1
1:A:348:VAL:HG13	1:A:348:VAL:O	0.45	2.11	5	1
1:A:367:HIS:O	1:A:367:HIS:ND1	0.45	2.49	11	1
1:A:319:CYS:CB	1:A:320:PRO:CD	0.45	2.94	16	1
1:A:359:GLU:OE1	1:A:360:GLU:N	0.45	2.49	17	1
1:A:345:GLN:OE1	1:A:371:CYS:SG	0.45	2.74	18	1
1:A:344:SER:O	1:A:345:GLN:OE1	0.45	2.35	18	1
1:A:311:LEU:O	1:A:312:LYS:O	0.45	2.35	10	1
1:A:309:ASN:ND2	1:A:311:LEU:HD21	0.45	2.25	14	1
1:A:315:TYR:CD1	1:A:315:TYR:N	0.45	2.81	10	2
1:A:297:CYS:SG	1:A:310:ASP:N	0.45	2.90	11	1
1:A:368:THR:O	1:A:369:LYS:CG	0.45	2.64	13	1
1:A:320:PRO:C	1:A:322:GLY:H	0.45	2.20	19	1
1:A:358:CYS:O	1:A:359:GLU:C	0.45	2.60	12	1
1:A:301:ASN:HD22	1:A:301:ASN:C	0.45	2.20	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:356:CYS:O	1:A:357:GLN:CD	0.45	2.60	15	2
1:A:298:LEU:CD2	1:A:298:LEU:N	0.45	2.78	16	1
1:A:359:GLU:C	1:A:361:GLY:H	0.45	2.20	6	1
1:A:324:GLN:CG	1:A:325:LEU:N	0.45	2.80	9	1
1:A:359:GLU:O	1:A:360:GLU:C	0.45	2.59	9	3
1:A:296:GLU:OE1	1:A:310:ASP:OD1	0.45	2.34	16	2
1:A:304:CYS:O	1:A:305:SER:C	0.45	2.60	19	6
1:A:295:ASN:C	1:A:297:CYS:N	0.45	2.75	10	2
1:A:310:ASP:OD1	1:A:310:ASP:C	0.45	2.60	10	3
1:A:296:GLU:OE1	1:A:310:ASP:OD2	0.44	2.35	6	6
1:A:367:HIS:N	1:A:367:HIS:ND1	0.44	2.56	2	1
1:A:365:ASP:OD1	1:A:365:ASP:C	0.44	2.61	8	1
1:A:298:LEU:N	1:A:298:LEU:HD22	0.44	2.26	16	1
1:A:296:GLU:OE2	1:A:310:ASP:OD2	0.44	2.34	19	1
1:A:302:GLY:C	1:A:315:TYR:OH	0.44	2.60	1	4
1:A:338:GLN:OE1	1:A:338:GLN:O	0.44	2.36	1	2
1:A:365:ASP:N	1:A:370:ALA:O	0.44	2.49	8	1
1:A:319:CYS:SG	1:A:320:PRO:CD	0.44	3.05	11	1
1:A:343:CYS:SG	1:A:347:CYS:CB	0.44	3.05	16	1
1:A:310:ASP:C	1:A:310:ASP:OD1	0.44	2.61	19	4
1:A:296:GLU:OE2	1:A:310:ASP:CG	0.44	2.60	7	1
1:A:298:LEU:H	1:A:298:LEU:HD22	0.44	1.71	16	1
1:A:364:LEU:C	1:A:364:LEU:CD1	0.44	2.90	2	1
1:A:349:ASN:OD1	1:A:349:ASN:C	0.44	2.61	4	4
1:A:336:GLU:N	1:A:349:ASN:ND2	0.44	2.65	19	1
1:A:338:GLN:O	1:A:338:GLN:CD	0.44	2.61	8	3
1:A:365:ASP:OD2	1:A:370:ALA:O	0.44	2.36	10	4
1:A:343:CYS:O	1:A:344:SER:C	0.44	2.60	20	3
1:A:316:GLU:CD	1:A:316:GLU:C	0.44	2.86	20	4
1:A:301:ASN:OD1	1:A:301:ASN:C	0.44	2.61	8	1
1:A:369:LYS:O	1:A:370:ALA:O	0.44	2.35	8	2
1:A:367:HIS:ND1	1:A:368:THR:OG1	0.44	2.44	7	1
1:A:333:ASP:OD2	1:A:350:LEU:O	0.43	2.36	9	12
1:A:334:ILE:O	1:A:336:GLU:OE2	0.43	2.36	11	6
1:A:309:ASN:C	1:A:309:ASN:ND2	0.43	2.75	8	2
1:A:345:GLN:CD	1:A:359:GLU:OE2	0.43	2.61	3	1
1:A:365:ASP:CG	1:A:368:THR:OG1	0.43	2.61	16	3
1:A:325:LEU:HD11	1:A:328:GLN:HA	0.43	1.90	15	1
1:A:299:ASP:O	1:A:300:ASN:O	0.43	2.37	17	1
1:A:324:GLN:OE1	1:A:333:ASP:O	0.43	2.37	4	1
1:A:365:ASP:OD1	1:A:370:ALA:O	0.43	2.37	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:319:CYS:O	1:A:320:PRO:C	0.43	2.61	17	1
1:A:345:GLN:OE1	1:A:359:GLU:OE1	0.43	2.36	3	1
1:A:307:VAL:O	1:A:318:LEU:N	0.43	2.51	4	1
1:A:333:ASP:OD2	1:A:349:ASN:OD1	0.43	2.36	10	2
1:A:330:ARG:O	1:A:331:CYS:O	0.43	2.36	6	2
1:A:301:ASN:O	1:A:301:ASN:CG	0.43	2.62	8	1
1:A:319:CYS:C	1:A:321:ASP:H	0.43	2.21	12	1
1:A:313:ILE:O	1:A:314:GLY:C	0.43	2.61	2	2
1:A:306:HIS:CD2	1:A:306:HIS:N	0.43	2.87	4	1
1:A:338:GLN:O	1:A:338:GLN:OE1	0.43	2.37	8	1
1:A:350:LEU:C	1:A:351:GLU:OE1	0.43	2.62	4	2
1:A:333:ASP:OD1	1:A:333:ASP:C	0.43	2.62	7	1
1:A:363:GLN:NE2	1:A:364:LEU:N	0.43	2.67	18	1
1:A:336:GLU:OE1	1:A:349:ASN:OD1	0.43	2.36	3	4
1:A:333:ASP:OD2	1:A:351:GLU:OE2	0.43	2.37	7	1
1:A:337:CYS:O	1:A:338:GLN:C	0.43	2.61	15	2
1:A:321:ASP:O	1:A:322:GLY:C	0.43	2.62	14	1
1:A:307:VAL:O	1:A:318:LEU:O	0.43	2.37	18	1
1:A:368:THR:O	1:A:369:LYS:C	0.43	2.62	1	2
1:A:365:ASP:CG	1:A:370:ALA:O	0.43	2.62	6	2
1:A:300:ASN:HD22	1:A:300:ASN:N	0.43	2.12	7	1
1:A:347:CYS:O	1:A:347:CYS:SG	0.43	2.77	11	2
1:A:336:GLU:N	1:A:336:GLU:CD	0.43	2.77	19	1
1:A:335:ASP:OD1	1:A:335:ASP:C	0.43	2.62	1	5
1:A:315:TYR:CD1	1:A:315:TYR:C	0.43	2.97	3	1
1:A:345:GLN:NE2	1:A:359:GLU:CD	0.43	2.77	3	1
1:A:299:ASP:O	1:A:300:ASN:C	0.43	2.62	5	3
1:A:302:GLY:O	1:A:329:ARG:NH2	0.43	2.51	10	2
1:A:322:GLY:C	1:A:323:PHE:CD1	0.43	2.97	15	1
1:A:365:ASP:OD2	1:A:369:LYS:C	0.42	2.62	10	1
1:A:319:CYS:C	1:A:320:PRO:O	0.42	2.61	13	1
1:A:309:ASN:C	1:A:309:ASN:HD22	0.42	2.21	17	2
1:A:356:CYS:C	1:A:357:GLN:CD	0.42	2.87	3	2
1:A:350:LEU:O	1:A:351:GLU:O	0.42	2.36	5	1
1:A:333:ASP:CG	1:A:350:LEU:O	0.42	2.62	8	2
1:A:351:GLU:CD	1:A:351:GLU:O	0.42	2.63	13	1
1:A:365:ASP:OD1	1:A:369:LYS:C	0.42	2.62	15	1
1:A:366:PRO:C	1:A:367:HIS:ND1	0.42	2.77	19	1
1:A:341:ASP:O	1:A:342:THR:C	0.42	2.62	8	5
1:A:338:GLN:CD	1:A:338:GLN:C	0.42	2.87	2	1
1:A:316:GLU:OE2	1:A:316:GLU:O	0.42	2.37	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:296:GLU:CD	1:A:310:ASP:OD1	0.42	2.63	7	1
1:A:303:GLY:O	1:A:304:CYS:O	0.42	2.36	9	1
1:A:361:GLY:C	1:A:362:PHE:CD1	0.42	2.97	15	1
1:A:351:GLU:O	1:A:351:GLU:OE2	0.42	2.37	13	1
1:A:345:GLN:HE22	1:A:364:LEU:CD2	0.42	2.26	18	1
1:A:340:PRO:C	1:A:341:ASP:OD1	0.42	2.63	12	1
1:A:356:CYS:C	1:A:357:GLN:OE1	0.42	2.62	12	1
1:A:365:ASP:OD1	1:A:370:ALA:C	0.42	2.62	5	1
1:A:351:GLU:OE1	1:A:351:GLU:N	0.42	2.52	4	1
1:A:301:ASN:CG	1:A:304:CYS:O	0.42	2.62	13	1
1:A:360:GLU:CD	1:A:360:GLU:N	0.42	2.78	16	1
1:A:306:HIS:NE2	1:A:330:ARG:NH2	0.42	2.68	18	1
1:A:363:GLN:CD	1:A:363:GLN:C	0.42	2.88	18	1
1:A:296:GLU:CD	1:A:310:ASP:OD2	0.42	2.62	3	1
1:A:301:ASN:O	1:A:302:GLY:C	0.42	2.63	3	1
1:A:337:CYS:O	1:A:337:CYS:SG	0.42	2.78	10	1
1:A:303:GLY:CA	1:A:329:ARG:NH1	0.42	2.83	19	1
1:A:344:SER:OG	1:A:358:CYS:SG	0.41	2.75	9	1
1:A:322:GLY:O	1:A:334:ILE:CG2	0.41	2.68	10	1
1:A:365:ASP:OD2	1:A:368:THR:OG1	0.41	2.37	19	2
1:A:330:ARG:O	1:A:331:CYS:CB	0.41	2.68	17	1
1:A:300:ASN:O	1:A:303:GLY:N	0.41	2.53	5	1
1:A:326:VAL:C	1:A:328:GLN:N	0.41	2.76	9	1
1:A:330:ARG:O	1:A:331:CYS:C	0.41	2.61	13	1
1:A:344:SER:C	1:A:345:GLN:CD	0.41	2.88	1	1
1:A:325:LEU:HD12	1:A:331:CYS:SG	0.41	2.56	19	1
1:A:355:LYS:CB	1:A:355:LYS:NZ	0.41	2.84	17	1
1:A:300:ASN:O	1:A:300:ASN:CG	0.41	2.64	8	1
1:A:345:GLN:C	1:A:345:GLN:CD	0.41	2.88	15	1
1:A:345:GLN:C	1:A:346:LEU:HD22	0.41	2.40	10	2
1:A:326:VAL:CG2	1:A:327:ALA:N	0.41	2.83	19	1
1:A:302:GLY:CA	1:A:315:TYR:CZ	0.41	3.03	3	1
1:A:345:GLN:NE2	1:A:358:CYS:SG	0.41	2.94	7	1
1:A:359:GLU:C	1:A:361:GLY:N	0.41	2.79	6	1
1:A:367:HIS:ND1	1:A:367:HIS:N	0.41	2.68	12	1
1:A:296:GLU:OE1	1:A:296:GLU:CA	0.41	2.69	13	1
1:A:354:TYR:CD1	1:A:354:TYR:N	0.41	2.89	17	1
1:A:345:GLN:OE1	1:A:359:GLU:CD	0.41	2.64	3	1
1:A:309:ASN:HD22	1:A:311:LEU:CD2	0.41	2.26	14	1
1:A:364:LEU:HD13	1:A:364:LEU:C	0.41	2.40	18	1
1:A:296:GLU:CD	1:A:296:GLU:H	0.41	2.21	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:307:VAL:O	1:A:307:VAL:CG1	0.40	2.69	6	2
1:A:326:VAL:HG22	1:A:327:ALA:N	0.40	2.31	9	1
1:A:351:GLU:OE1	1:A:351:GLU:CA	0.40	2.69	9	1
1:A:364:LEU:O	1:A:365:ASP:C	0.40	2.64	15	1
1:A:321:ASP:OD1	1:A:321:ASP:C	0.40	2.64	2	1
1:A:336:GLU:O	1:A:342:THR:OG1	0.40	2.35	20	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	77/80 (96%)	51±3 (67±4%)	18±3 (23±4%)	8±2 (11±3%)	1	9
All	All	1540/1600 (96%)	1025 (67%)	353 (23%)	162 (11%)	1	9

All 32 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	328	GLN	20
1	A	321	ASP	15
1	A	369	LYS	13
1	A	320	PRO	12
1	A	312	LYS	11
1	A	314	GLY	10
1	A	313	ILE	9
1	A	303	GLY	5
1	A	361	GLY	5
1	A	331	CYS	5
1	A	345	GLN	5
1	A	370	ALA	5
1	A	295	ASN	5
1	A	300	ASN	5
1	A	326	VAL	4
1	A	327	ALA	4

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Mol	Chain	Res	Type	Models (Total)
1	A	366	PRO	4
1	A	322	GLY	3
1	A	359	GLU	3
1	A	315	TYR	2
1	A	310	ASP	2
1	A	360	GLU	2
1	A	298	LEU	2
1	A	338	GLN	2
1	A	344	SER	2
1	A	351	GLU	1
1	A	301	ASN	1
1	A	302	GLY	1
1	A	305	SER	1
1	A	304	CYS	1
1	A	296	GLU	1
1	A	299	ASP	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	69/70 (99%)	62±2 (89±4%)	7±2 (11±4%)	9	52
All	All	1380/1400 (99%)	1234 (89%)	146 (11%)	9	52

All 42 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	318	LEU	13
1	A	319	CYS	11
1	A	331	CYS	10
1	A	329	ARG	9
1	A	358	CYS	9
1	A	368	THR	7
1	A	330	ARG	6
1	A	343	CYS	6
1	A	297	CYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	301	ASN	4
1	A	346	LEU	4
1	A	355	LYS	4
1	A	357	GLN	4
1	A	369	LYS	4
1	A	324	GLN	3
1	A	316	GLU	3
1	A	359	GLU	3
1	A	296	GLU	3
1	A	295	ASN	3
1	A	351	GLU	3
1	A	328	GLN	3
1	A	300	ASN	2
1	A	364	LEU	2
1	A	304	CYS	2
1	A	310	ASP	2
1	A	356	CYS	2
1	A	372	LYS	2
1	A	321	ASP	2
1	A	348	VAL	2
1	A	313	ILE	1
1	A	367	HIS	1
1	A	308	CYS	1
1	A	344	SER	1
1	A	347	CYS	1
1	A	305	SER	1
1	A	309	ASN	1
1	A	312	LYS	1
1	A	365	ASP	1
1	A	371	CYS	1
1	A	339	ASP	1
1	A	338	GLN	1
1	A	307	VAL	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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