



Full wwPDB NMR Structure Validation Report ⓘ

Oct 23, 2021 – 05:19 PM EDT

PDB ID : 1BWM
Title : A SINGLE-CHAIN T CELL RECEPTOR
Authors : Hare, B.J.; Wyss, D.F.; Reinherz, E.L.; Wagner, G.
Deposited on : 1998-09-23

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

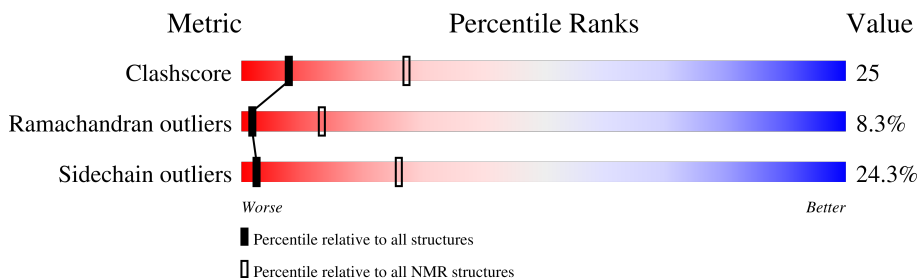
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	249	

2 Ensemble composition and analysis

This entry contains 15 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 7 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:3-A:63, A:65-A:96, A:105-A:116, A:301-A:359, A:361-A:393, A:399-A:414 (213)	0.85	15

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

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

The models can be grouped into 2 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3709 atoms, of which 1807 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10)).

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	249	3709	1185	1807	334	378	5	0

There is a discrepancy between the modelled and reference sequences:

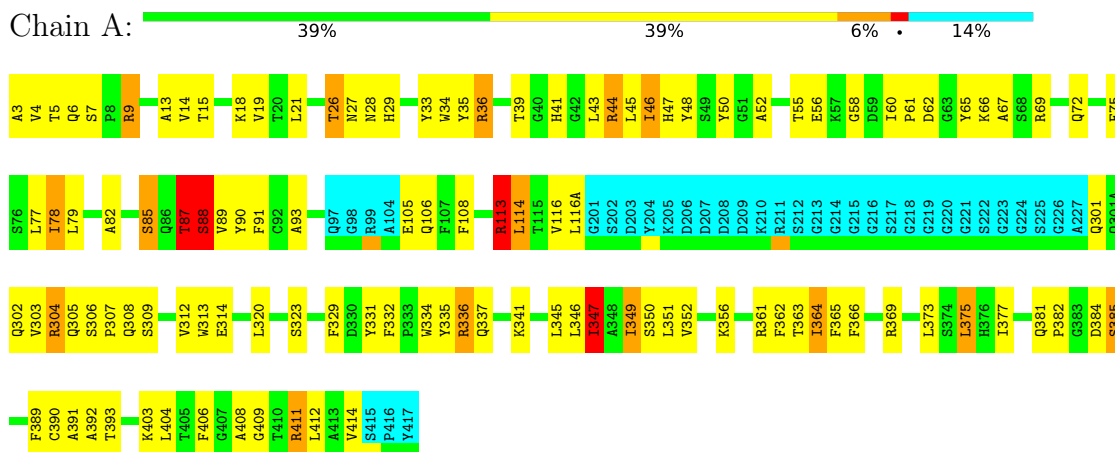
Chain	Residue	Modelled	Actual	Comment	Reference
A	415	SER	CYS	engineered mutation	GB 5724764

4 Residue-property plots i

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

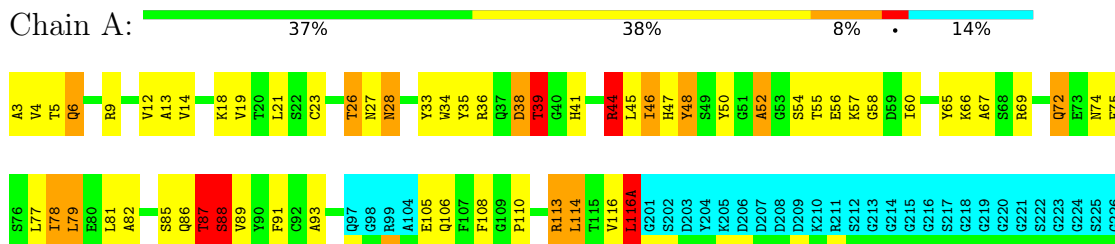


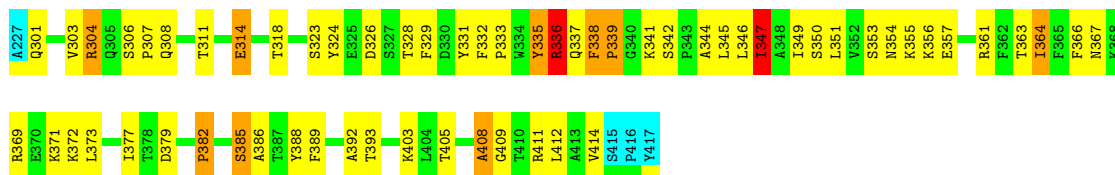
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

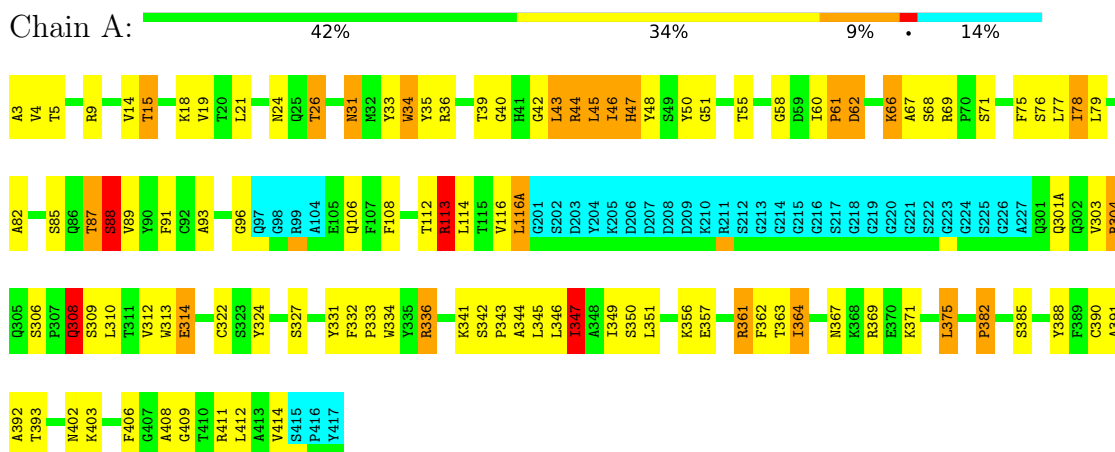
- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))





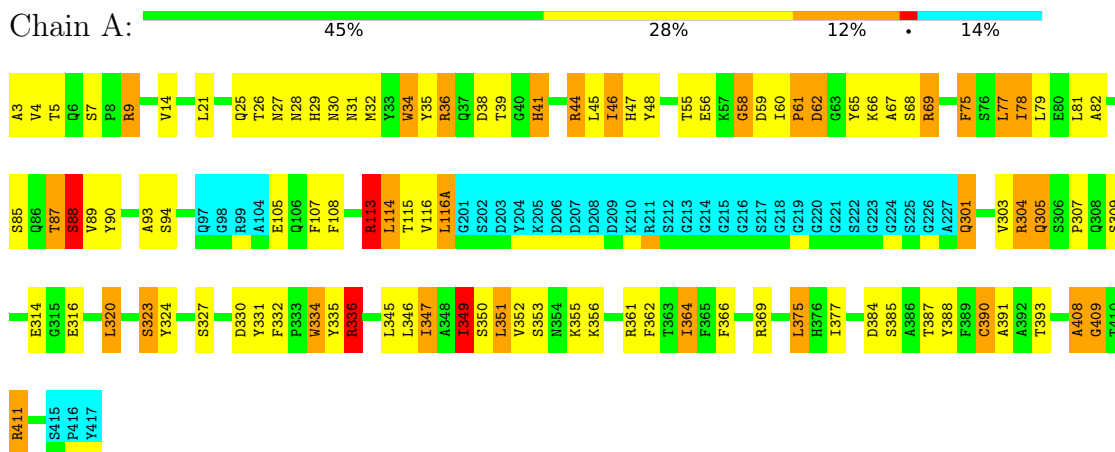
4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



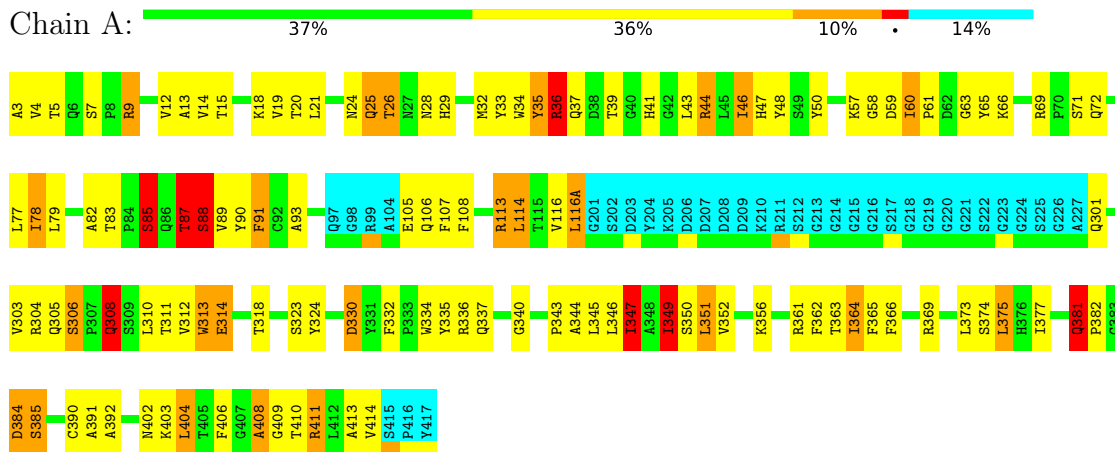
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



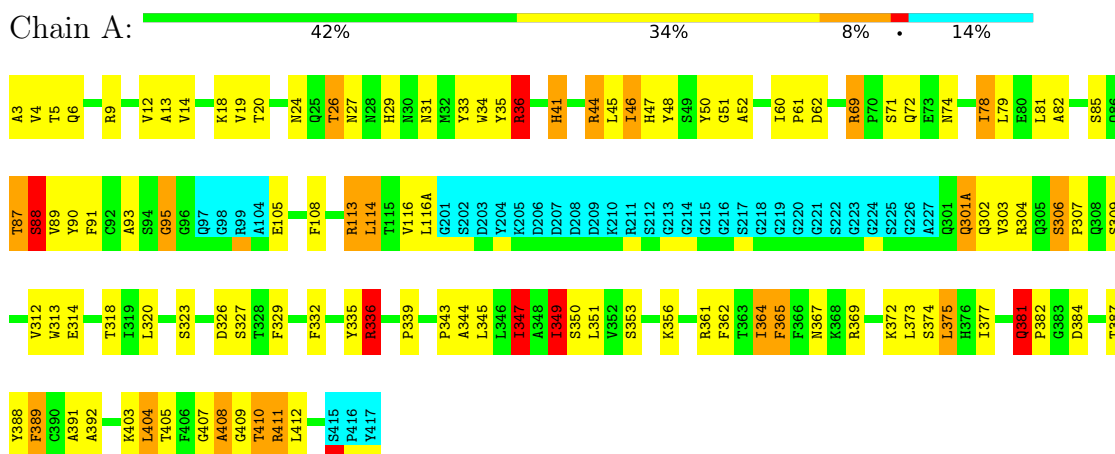
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



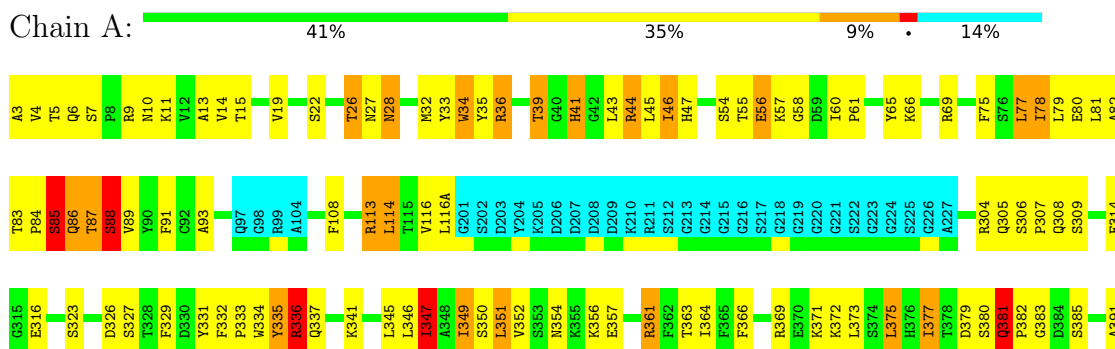
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

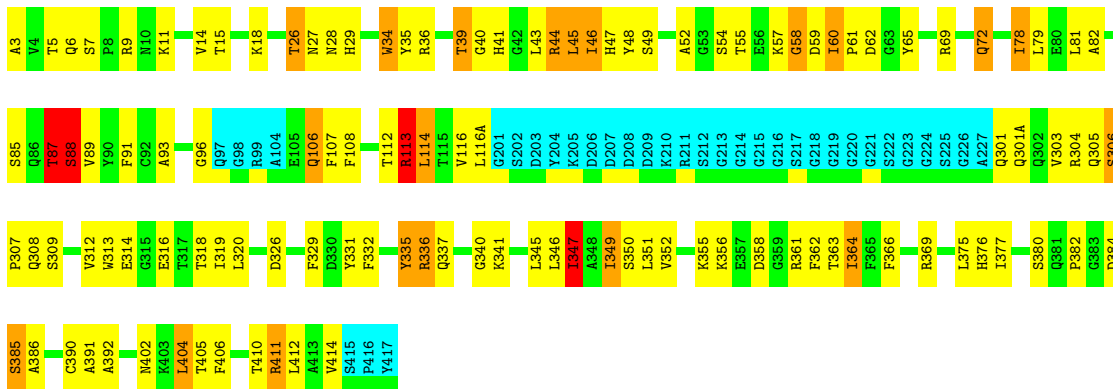




4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

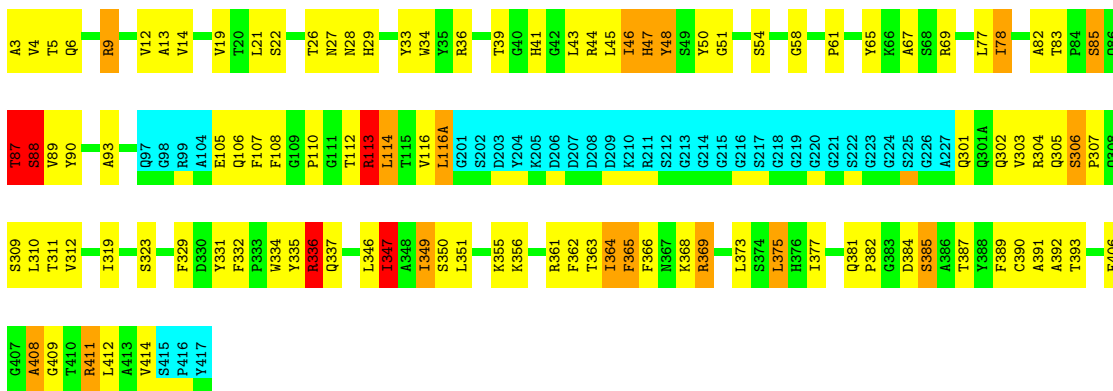
Chain A: 39% 37% 8% 14%



4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

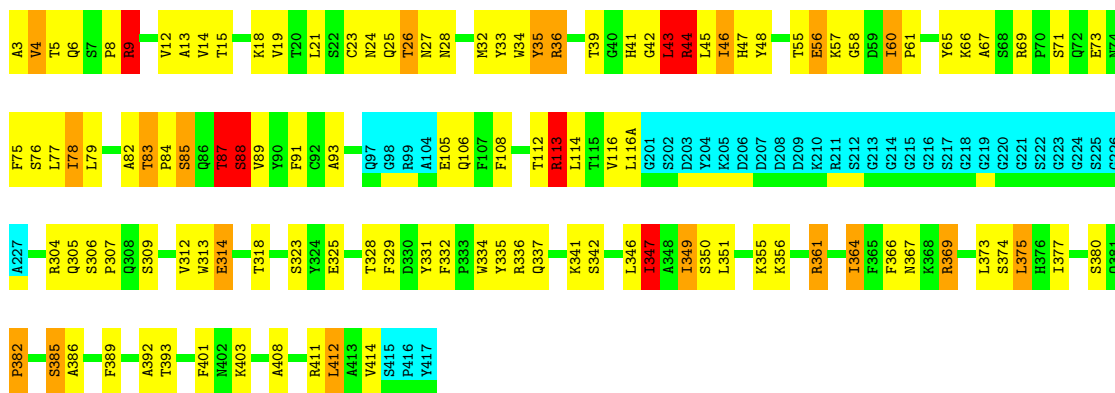
Chain A: 43% 35% 7% 14%



4.2.9 Score per residue for model 9

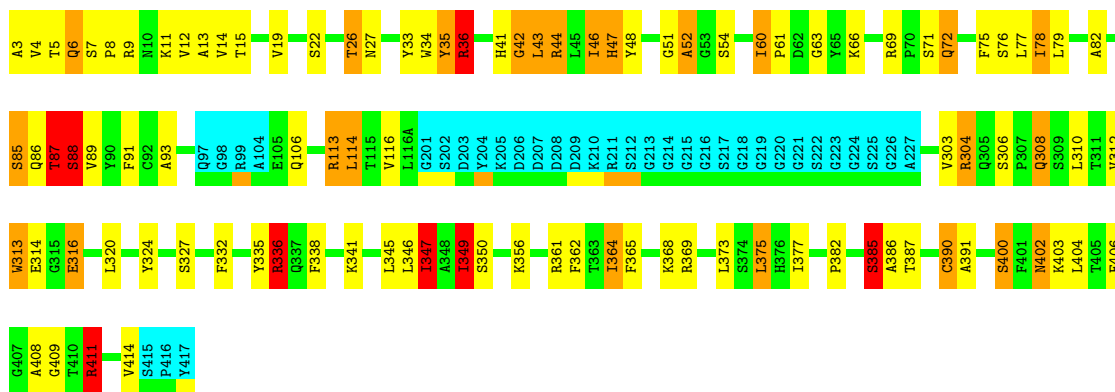
- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

Chain A: 39% 37% 8% 14%



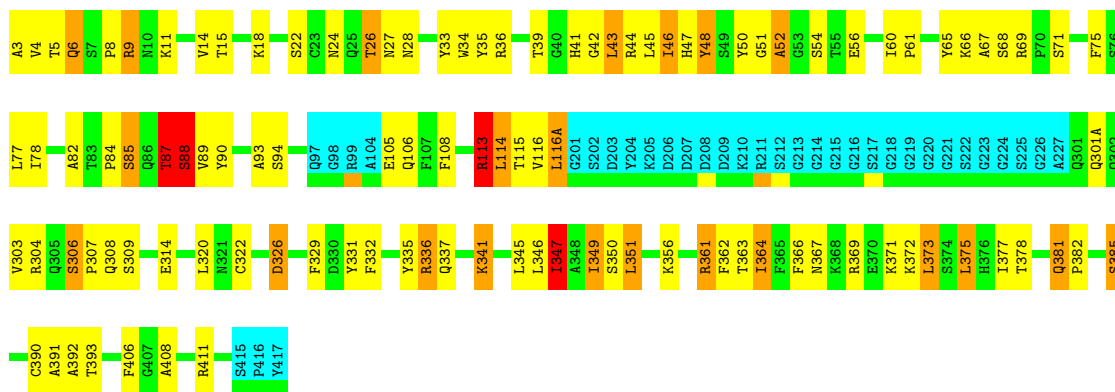
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



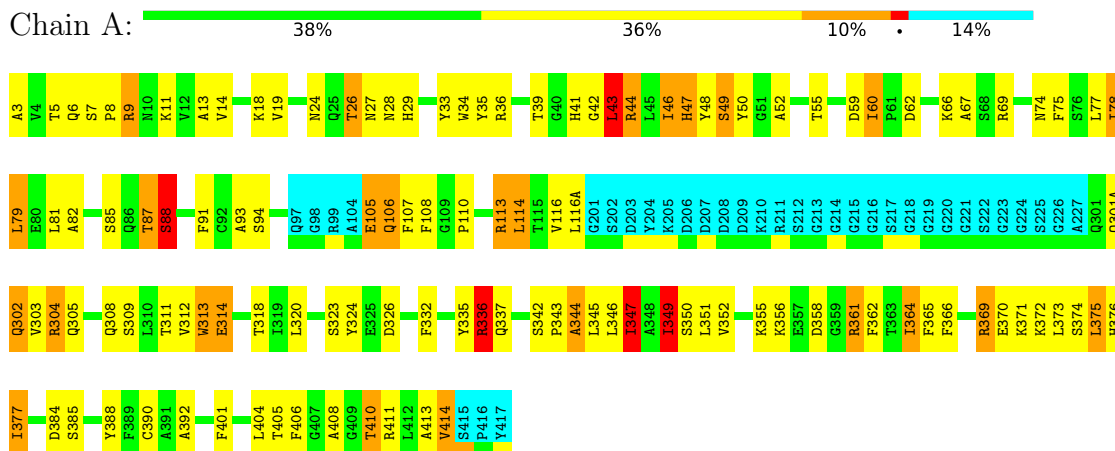
4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



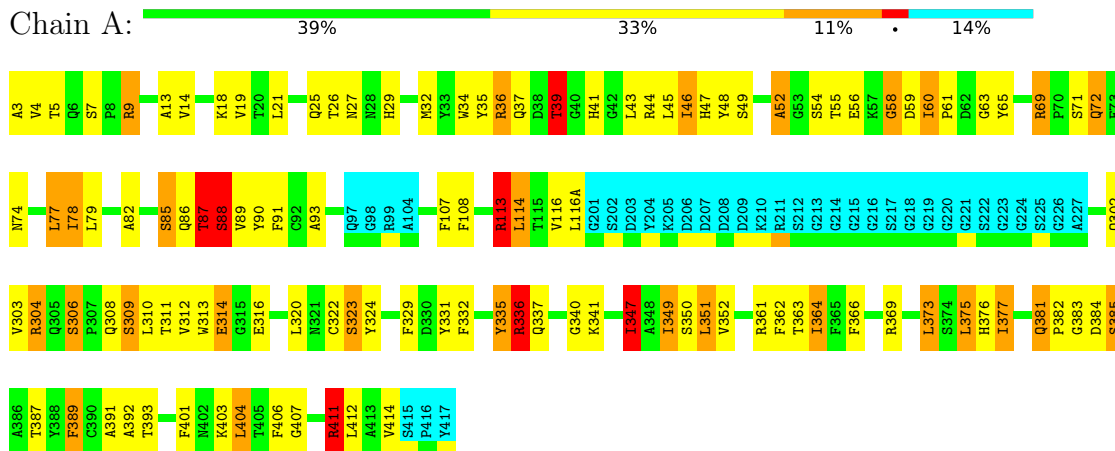
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



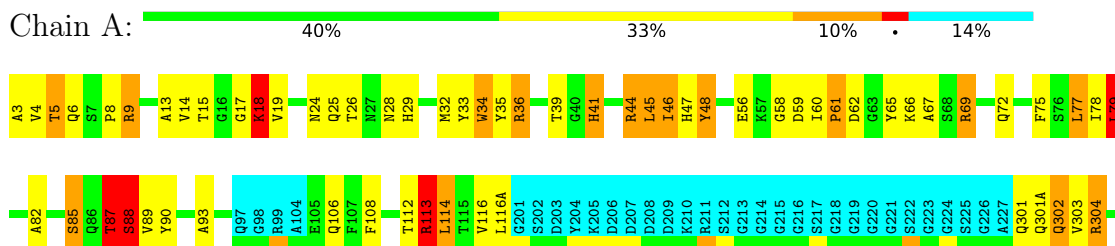
4.2.13 Score per residue for model 13

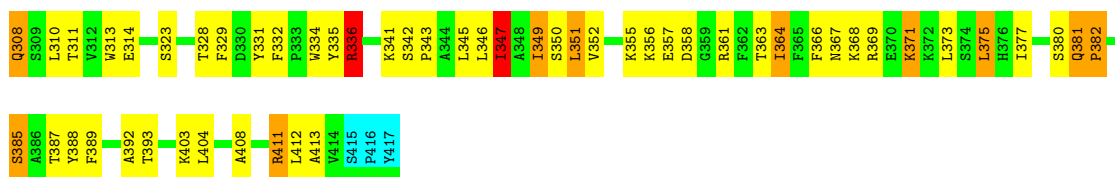
- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))



4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

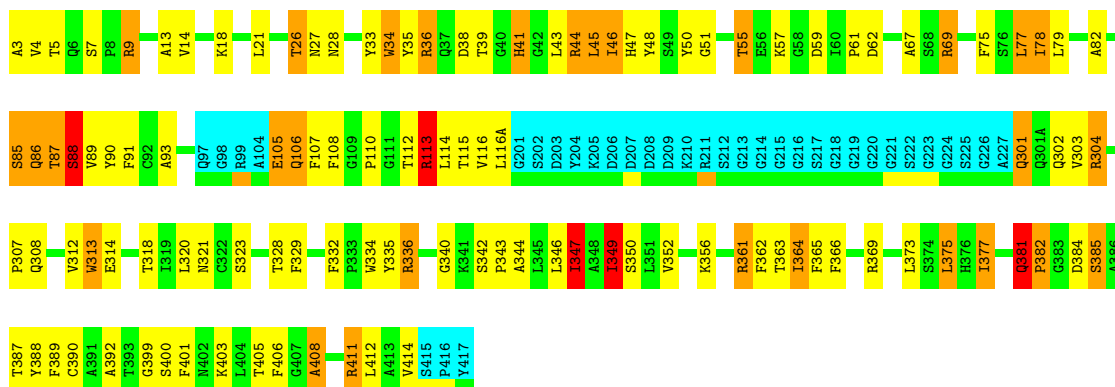




4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: PROTEIN (ALPHA-BETA T CELL RECEPTOR (TCR) (D10))

Chain A: 40% 33% 12% 14%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 80 calculated structures, 15 were deposited, based on the following criterion: *NO NOE DISTANCE VIOLATION GREATER THAN 0.5 Å, NO DIHEDRAL VIOLATION GREATER THAN 5 DEGREES*.

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](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	10.0±0.0
All	All	0	150

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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	A	9	ARG	Sidechain	15
1	A	36	ARG	Sidechain	15
1	A	44	ARG	Sidechain	15
1	A	69	ARG	Sidechain	15
1	A	113	ARG	Sidechain	15
1	A	304	ARG	Sidechain	15
1	A	336	ARG	Sidechain	15
1	A	361	ARG	Sidechain	15
1	A	369	ARG	Sidechain	15
1	A	411	ARG	Sidechain	15

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1683	1623	1620	84±8
All	All	25245	24345	24300	1253

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:HG11	1:A:114:LEU:HD22	1.13	1.16	14	1
1:A:82:ALA:HB1	1:A:116:VAL:HG21	0.97	1.36	13	6
1:A:318:THR:HG21	1:A:412:LEU:HD11	0.95	1.36	9	2
1:A:311:THR:HG23	1:A:413:ALA:HB3	0.94	1.37	12	2
1:A:19:VAL:HG13	1:A:114:LEU:HD21	0.93	1.40	4	8
1:A:82:ALA:HB3	1:A:116:VAL:HG21	0.93	1.39	9	9
1:A:65:TYR:CZ	1:A:79:LEU:HD21	0.90	2.02	6	1
1:A:93:ALA:HB2	1:A:108:PHE:CE1	0.87	2.05	1	7
1:A:77:LEU:HD22	1:A:78:ILE:N	0.85	1.86	15	1
1:A:331:TYR:CE1	1:A:393:THR:HG21	0.83	2.08	11	3
1:A:35:TYR:CE1	1:A:45:LEU:HD12	0.83	2.08	7	4
1:A:19:VAL:HG23	1:A:79:LEU:HD22	0.83	1.51	1	2
1:A:45:LEU:C	1:A:46:ILE:HD13	0.83	1.94	11	1
1:A:19:VAL:HG11	1:A:114:LEU:CD2	0.81	2.04	14	1
1:A:351:LEU:HD12	1:A:373:LEU:HD21	0.81	1.52	14	2
1:A:47:HIS:CD2	1:A:77:LEU:HD22	0.81	2.11	11	2
1:A:82:ALA:HB3	1:A:116:VAL:HG11	0.80	1.54	3	5
1:A:3:ALA:O	1:A:5:THR:HG23	0.79	1.77	15	10
1:A:41:HIS:CD2	1:A:408:ALA:HB1	0.79	2.12	15	6
1:A:19:VAL:CG2	1:A:79:LEU:HD22	0.79	2.08	1	2
1:A:303:VAL:HG11	1:A:390:CYS:O	0.79	1.78	2	9
1:A:43:LEU:HD13	1:A:406:PHE:CG	0.79	2.13	4	1
1:A:82:ALA:CB	1:A:116:VAL:HG21	0.79	2.08	5	14
1:A:19:VAL:HG13	1:A:114:LEU:CD2	0.79	2.08	8	7
1:A:3:ALA:CA	1:A:26:THR:HG22	0.78	2.08	9	1
1:A:116(A):LEU:C	1:A:116(A):LEU:HD22	0.77	2.00	3	1
1:A:77:LEU:O	1:A:77:LEU:HD13	0.77	1.77	15	1
1:A:351:LEU:HD13	1:A:373:LEU:CD2	0.77	2.10	1	1
1:A:60:ILE:O	1:A:60:ILE:HD12	0.77	1.79	3	6
1:A:93:ALA:HB2	1:A:108:PHE:CD1	0.77	2.13	8	7
1:A:65:TYR:CE2	1:A:79:LEU:HD21	0.76	2.14	6	1
1:A:47:HIS:NE2	1:A:77:LEU:HD13	0.76	1.94	11	1
1:A:312:VAL:CG1	1:A:414:VAL:HG22	0.76	2.09	10	1
1:A:14:VAL:O	1:A:116:VAL:HG13	0.76	1.80	7	15
1:A:41:HIS:CE1	1:A:408:ALA:HB1	0.76	2.16	8	1
1:A:15:THR:OG1	1:A:116(A):LEU:HD22	0.76	1.79	6	1
1:A:3:ALA:HA	1:A:26:THR:HG22	0.75	1.59	9	1
1:A:87:THR:HG23	1:A:116:VAL:HG23	0.73	1.60	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ALA:O	1:A:116:VAL:HG11	0.73	1.83	8	4
1:A:3:ALA:O	1:A:5:THR:HG22	0.73	1.84	14	1
1:A:83:THR:HG22	1:A:86:GLN:HG2	0.73	1.60	6	1
1:A:318:THR:HG21	1:A:412:LEU:CD1	0.73	2.12	9	1
1:A:356:LYS:O	1:A:364:ILE:HD12	0.73	1.83	11	5
1:A:89:VAL:HG22	1:A:113:ARG:CB	0.73	2.14	2	9
1:A:311:THR:HG23	1:A:413:ALA:CB	0.72	2.14	12	2
1:A:82:ALA:HB1	1:A:116:VAL:CG2	0.72	2.14	13	1
1:A:79:LEU:HD13	1:A:90:TYR:CE1	0.72	2.20	14	1
1:A:46:ILE:HD13	1:A:46:ILE:N	0.72	1.99	11	14
1:A:381:GLN:O	1:A:414:VAL:HG11	0.72	1.85	15	1
1:A:4:VAL:HG21	1:A:107:PHE:O	0.72	1.84	13	1
1:A:351:LEU:HD21	1:A:366:PHE:CE1	0.71	2.20	6	8
1:A:391:ALA:HB2	1:A:406:PHE:CD1	0.71	2.18	6	2
1:A:76:SER:O	1:A:77:LEU:HD22	0.71	1.85	9	3
1:A:364:ILE:HD13	1:A:364:ILE:N	0.71	2.01	1	9
1:A:331:TYR:CE2	1:A:393:THR:HG21	0.71	2.19	8	2
1:A:346:LEU:N	1:A:346:LEU:HD22	0.71	2.01	3	1
1:A:13:ALA:HB3	1:A:116:VAL:HG22	0.70	1.62	13	6
1:A:331:TYR:CZ	1:A:393:THR:HG21	0.70	2.21	9	6
1:A:347:ILE:N	1:A:347:ILE:HD13	0.70	2.01	2	13
1:A:47:HIS:CE1	1:A:67:ALA:HB2	0.70	2.21	1	2
1:A:336:ARG:HB2	1:A:346:LEU:HD21	0.70	1.62	3	3
1:A:305:GLN:OE1	1:A:410:THR:HG23	0.69	1.88	12	1
1:A:67:ALA:HB2	1:A:77:LEU:HD13	0.69	1.62	3	1
1:A:89:VAL:HG22	1:A:113:ARG:HB2	0.69	1.63	4	3
1:A:93:ALA:HB2	1:A:108:PHE:HB3	0.69	1.64	15	4
1:A:302:GLN:HG3	1:A:405:THR:HG21	0.69	1.63	5	1
1:A:306:SER:O	1:A:410:THR:HG21	0.69	1.88	5	1
1:A:41:HIS:HA	1:A:408:ALA:HB2	0.68	1.64	1	1
1:A:318:THR:CG2	1:A:412:LEU:HD11	0.68	2.15	9	1
1:A:336:ARG:HB2	1:A:346:LEU:HD11	0.68	1.65	2	8
1:A:362:PHE:CE1	1:A:377:ILE:HD13	0.68	2.24	11	1
1:A:114:LEU:HD12	1:A:115:THR:N	0.68	2.04	11	3
1:A:35:TYR:CE2	1:A:43:LEU:HD22	0.68	2.24	9	2
1:A:35:TYR:HB3	1:A:43:LEU:HD21	0.67	1.64	2	1
1:A:387:THR:HG22	1:A:411:ARG:HG3	0.67	1.65	14	3
1:A:338:PHE:CE1	1:A:346:LEU:HD21	0.67	2.25	1	1
1:A:4:VAL:HG23	1:A:24:ASN:O	0.67	1.89	4	4
1:A:87:THR:CG2	1:A:116:VAL:HG23	0.66	2.19	3	8
1:A:311:THR:CG2	1:A:413:ALA:HB3	0.66	2.17	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:PHE:CD1	1:A:392:ALA:HB2	0.66	2.25	2	6
1:A:77:LEU:HD13	1:A:77:LEU:C	0.66	2.09	15	1
1:A:332:PHE:CE2	1:A:392:ALA:HB2	0.66	2.25	1	6
1:A:79:LEU:HD22	1:A:90:TYR:CE2	0.66	2.26	14	1
1:A:89:VAL:HG13	1:A:113:ARG:HB3	0.66	1.67	4	4
1:A:385:SER:OG	1:A:414:VAL:HG13	0.66	1.91	9	1
1:A:78:ILE:N	1:A:78:ILE:HD13	0.65	2.06	12	8
1:A:60:ILE:HD13	1:A:60:ILE:N	0.65	2.06	4	3
1:A:78:ILE:O	1:A:79:LEU:HD22	0.65	1.90	13	2
1:A:79:LEU:HD11	1:A:114:LEU:HD21	0.65	1.67	14	1
1:A:335:TYR:CB	1:A:345:LEU:HA	0.65	2.22	5	2
1:A:3:ALA:CB	1:A:26:THR:HG22	0.65	2.22	9	1
1:A:77:LEU:O	1:A:78:ILE:HD12	0.64	1.92	14	1
1:A:93:ALA:HB1	1:A:106:GLN:HB3	0.64	1.70	12	3
1:A:349:ILE:H	1:A:349:ILE:HD13	0.64	1.53	3	6
1:A:67:ALA:HB2	1:A:77:LEU:HD23	0.64	1.70	15	1
1:A:314:GLU:HB2	1:A:414:VAL:HG11	0.64	1.69	12	1
1:A:3:ALA:HA	1:A:26:THR:HG23	0.63	1.70	2	7
1:A:391:ALA:HB2	1:A:406:PHE:CD2	0.63	2.28	4	3
1:A:93:ALA:HB1	1:A:106:GLN:HG2	0.63	1.71	7	1
1:A:46:ILE:HD13	1:A:46:ILE:H	0.62	1.54	9	13
1:A:347:ILE:HD12	1:A:362:PHE:CZ	0.62	2.30	2	3
1:A:35:TYR:CE1	1:A:45:LEU:HD13	0.62	2.30	1	1
1:A:351:LEU:HD12	1:A:373:LEU:CD2	0.62	2.24	14	1
1:A:5:THR:OG1	1:A:6:GLN:N	0.62	2.33	14	1
1:A:351:LEU:HD23	1:A:351:LEU:O	0.62	1.95	8	2
1:A:79:LEU:CD1	1:A:114:LEU:HD21	0.62	2.24	14	1
1:A:388:TYR:CE1	1:A:412:LEU:HD21	0.62	2.30	14	1
1:A:66:LYS:O	1:A:77:LEU:HD13	0.61	1.95	9	2
1:A:45:LEU:HD21	1:A:48:TYR:CD1	0.61	2.31	9	1
1:A:59:ASP:HB3	1:A:60:ILE:HD13	0.61	1.70	13	3
1:A:87:THR:OG1	1:A:88:SER:N	0.61	2.32	11	2
1:A:312:VAL:HG11	1:A:414:VAL:HG22	0.61	1.71	10	1
1:A:346:LEU:HB2	1:A:347:ILE:HD13	0.61	1.72	6	8
1:A:375:LEU:HD12	1:A:376:HIS:N	0.61	2.11	7	1
1:A:387:THR:HG22	1:A:411:ARG:HG2	0.61	1.73	10	2
1:A:332:PHE:CE1	1:A:392:ALA:HB2	0.60	2.30	2	3
1:A:404:LEU:HD22	1:A:406:PHE:CE1	0.60	2.32	10	1
1:A:303:VAL:HG12	1:A:407:GLY:CA	0.60	2.27	13	1
1:A:347:ILE:HD13	1:A:347:ILE:H	0.60	1.56	13	13
1:A:65:TYR:CE2	1:A:79:LEU:HD11	0.60	2.31	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:303:VAL:HG21	1:A:405:THR:O	0.59	1.97	1	2
1:A:347:ILE:H	1:A:347:ILE:HD13	0.59	1.58	5	2
1:A:105:GLU:CB	1:A:345:LEU:HD22	0.59	2.27	5	1
1:A:89:VAL:HG13	1:A:113:ARG:HG2	0.59	1.73	6	1
1:A:347:ILE:HD13	1:A:347:ILE:N	0.59	2.11	5	2
1:A:77:LEU:HD22	1:A:77:LEU:C	0.59	2.18	15	1
1:A:377:ILE:HG23	1:A:377:ILE:O	0.59	1.98	4	12
1:A:411:ARG:O	1:A:412:LEU:HD22	0.58	1.96	13	1
1:A:350:SER:C	1:A:351:LEU:HD23	0.58	2.17	4	1
1:A:385:SER:HB2	1:A:414:VAL:HG23	0.58	1.75	7	1
1:A:79:LEU:HD22	1:A:90:TYR:CZ	0.58	2.33	14	1
1:A:338:PHE:CZ	1:A:344:ALA:HB3	0.58	2.33	1	1
1:A:78:ILE:H	1:A:78:ILE:HD13	0.58	1.59	10	3
1:A:87:THR:O	1:A:88:SER:CB	0.58	2.51	11	15
1:A:336:ARG:NE	1:A:386:ALA:HB1	0.58	2.13	10	1
1:A:35:TYR:OH	1:A:404:LEU:HD22	0.58	1.99	12	2
1:A:26:THR:O	1:A:26:THR:HG23	0.58	1.99	9	1
1:A:351:LEU:HD11	1:A:366:PHE:CD1	0.57	2.34	1	1
1:A:335:TYR:CE2	1:A:345:LEU:HD13	0.57	2.33	14	2
1:A:351:LEU:HD13	1:A:373:LEU:HD23	0.57	1.76	1	1
1:A:332:PHE:CE1	1:A:351:LEU:HD13	0.57	2.33	11	1
1:A:335:TYR:O	1:A:336:ARG:HB2	0.57	1.97	5	2
1:A:46:ILE:N	1:A:46:ILE:CD1	0.57	2.65	11	8
1:A:310:LEU:HD23	1:A:311:THR:N	0.57	2.15	13	2
1:A:14:VAL:C	1:A:116:VAL:HG13	0.57	2.20	14	5
1:A:351:LEU:HD12	1:A:373:LEU:HD11	0.57	1.77	8	1
1:A:19:VAL:HG23	1:A:79:LEU:CD2	0.56	2.27	1	2
1:A:55:THR:O	1:A:56:GLU:HB3	0.56	2.00	9	1
1:A:332:PHE:CD2	1:A:392:ALA:HB2	0.56	2.35	11	3
1:A:79:LEU:HD13	1:A:90:TYR:CZ	0.56	2.35	14	1
1:A:391:ALA:HB1	1:A:404:LEU:CD2	0.56	2.31	10	1
1:A:41:HIS:NE2	1:A:408:ALA:HB1	0.56	2.15	15	1
1:A:349:ILE:HD13	1:A:349:ILE:N	0.56	2.16	3	6
1:A:364:ILE:N	1:A:364:ILE:CD1	0.56	2.67	1	9
1:A:89:VAL:HG22	1:A:113:ARG:HB3	0.56	1.77	3	3
1:A:335:TYR:CZ	1:A:345:LEU:HD12	0.55	2.36	7	1
1:A:352:VAL:HG22	1:A:352:VAL:O	0.55	2.02	13	8
1:A:35:TYR:CZ	1:A:45:LEU:HD12	0.55	2.36	3	3
1:A:60:ILE:N	1:A:61:PRO:CD	0.55	2.69	5	9
1:A:78:ILE:HD13	1:A:78:ILE:H	0.55	1.60	12	5
1:A:345:LEU:HD23	1:A:346:LEU:N	0.55	2.16	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:THR:HG22	1:A:114:LEU:O	0.55	2.02	13	7
1:A:43:LEU:HD13	1:A:406:PHE:CB	0.55	2.32	4	1
1:A:363:THR:HG23	1:A:363:THR:O	0.55	2.02	11	4
1:A:60:ILE:HD13	1:A:60:ILE:H	0.55	1.62	4	3
1:A:343:PRO:O	1:A:344:ALA:HB2	0.54	2.02	12	5
1:A:55:THR:O	1:A:56:GLU:CB	0.54	2.55	9	1
1:A:52:ALA:HB2	1:A:72:GLN:HB2	0.54	1.80	5	3
1:A:50:TYR:CD1	1:A:50:TYR:N	0.54	2.75	12	3
1:A:87:THR:HG21	1:A:116:VAL:HG23	0.54	1.79	5	4
1:A:391:ALA:HB2	1:A:406:PHE:CE1	0.54	2.37	6	1
1:A:116(A):LEU:C	1:A:116(A):LEU:CD2	0.54	2.75	3	1
1:A:35:TYR:HB3	1:A:43:LEU:HD22	0.54	1.79	6	2
1:A:116(A):LEU:CD1	1:A:116(A):LEU:N	0.54	2.71	3	1
1:A:335:TYR:C	1:A:335:TYR:CD1	0.54	2.81	13	1
1:A:79:LEU:C	1:A:79:LEU:HD23	0.54	2.23	12	2
1:A:347:ILE:N	1:A:347:ILE:CD1	0.54	2.71	9	15
1:A:78:ILE:HD13	1:A:78:ILE:N	0.54	2.18	10	3
1:A:52:ALA:HB2	1:A:72:GLN:CG	0.53	2.33	10	1
1:A:93:ALA:HB2	1:A:108:PHE:HD2	0.53	1.64	5	1
1:A:385:SER:CB	1:A:414:VAL:HG23	0.53	2.33	8	1
1:A:66:LYS:CB	1:A:78:ILE:HD11	0.53	2.34	2	1
1:A:303:VAL:HA	1:A:323:SER:O	0.53	2.03	5	5
1:A:334:TRP:CD1	1:A:334:TRP:O	0.53	2.62	3	1
1:A:75:PHE:CE2	1:A:77:LEU:HD23	0.53	2.39	1	1
1:A:385:SER:O	1:A:386:ALA:HB2	0.53	2.04	9	4
1:A:362:PHE:CD1	1:A:377:ILE:HD13	0.53	2.38	11	1
1:A:78:ILE:CG2	1:A:79:LEU:N	0.53	2.71	14	1
1:A:349:ILE:HD12	1:A:373:LEU:HD22	0.53	1.81	14	1
1:A:55:THR:HG23	1:A:56:GLU:HG3	0.52	1.81	6	1
1:A:33:TYR:CD1	1:A:48:TYR:CZ	0.52	2.98	11	2
1:A:3:ALA:CA	1:A:26:THR:HG23	0.52	2.34	2	3
1:A:312:VAL:HG22	1:A:318:THR:HG23	0.52	1.80	12	1
1:A:60:ILE:N	1:A:61:PRO:HD3	0.52	2.18	5	7
1:A:47:HIS:CE1	1:A:65:TYR:CE1	0.52	2.98	8	1
1:A:387:THR:HG22	1:A:411:ARG:HB2	0.52	1.81	8	1
1:A:303:VAL:HG13	1:A:322:CYS:SG	0.52	2.44	2	1
1:A:389:PHE:CD2	1:A:406:PHE:CE2	0.52	2.97	13	1
1:A:346:LEU:N	1:A:346:LEU:CD2	0.52	2.72	3	1
1:A:35:TYR:CZ	1:A:406:PHE:CE1	0.52	2.98	13	1
1:A:351:LEU:CD1	1:A:373:LEU:HD11	0.52	2.34	13	1
1:A:21:LEU:HD21	1:A:112:THR:HG21	0.52	1.80	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:303:VAL:HG12	1:A:407:GLY:HA3	0.52	1.81	13	1
1:A:387:THR:HG22	1:A:411:ARG:HD2	0.52	1.81	13	1
1:A:60:ILE:O	1:A:60:ILE:CD1	0.52	2.57	3	4
1:A:381:GLN:CB	1:A:382:PRO:HD3	0.52	2.35	6	6
1:A:383:GLY:N	1:A:414:VAL:HG21	0.51	2.20	13	1
1:A:93:ALA:CB	1:A:108:PHE:HB3	0.51	2.36	4	4
1:A:351:LEU:HD11	1:A:373:LEU:HD11	0.51	1.81	13	1
1:A:381:GLN:CB	1:A:382:PRO:CD	0.51	2.88	5	6
1:A:362:PHE:CD1	1:A:375:LEU:HD11	0.51	2.41	13	5
1:A:349:ILE:HG12	1:A:350:SER:N	0.51	2.20	4	6
1:A:39:THR:O	1:A:41:HIS:N	0.51	2.43	7	2
1:A:78:ILE:N	1:A:78:ILE:CD1	0.51	2.74	12	9
1:A:43:LEU:C	1:A:43:LEU:HD13	0.51	2.26	11	2
1:A:66:LYS:HB3	1:A:78:ILE:HD11	0.51	1.83	2	2
1:A:35:TYR:CD2	1:A:43:LEU:HD13	0.51	2.40	10	1
1:A:46:ILE:HG12	1:A:47:HIS:N	0.50	2.21	10	13
1:A:363:THR:C	1:A:364:ILE:HD13	0.50	2.26	1	3
1:A:115:THR:HG22	1:A:116(A):LEU:HD12	0.50	1.83	3	1
1:A:306:SER:N	1:A:307:PRO:CD	0.50	2.73	7	3
1:A:4:VAL:HG11	1:A:107:PHE:HB3	0.50	1.82	13	1
1:A:78:ILE:C	1:A:79:LEU:HD23	0.50	2.26	14	1
1:A:382:PRO:HA	1:A:414:VAL:HG21	0.50	1.82	9	2
1:A:312:VAL:HG11	1:A:412:LEU:HD13	0.50	1.84	8	1
1:A:389:PHE:CE2	1:A:391:ALA:HB2	0.50	2.41	13	1
1:A:386:ALA:HB3	1:A:388:TYR:CE1	0.50	2.40	1	1
1:A:326:ASP:OD1	1:A:328:THR:HG22	0.50	2.07	1	1
1:A:332:PHE:HB2	1:A:349:ILE:HD11	0.50	1.83	13	13
1:A:382:PRO:HA	1:A:414:VAL:HG11	0.50	1.82	2	1
1:A:4:VAL:C	1:A:5:THR:HG22	0.50	2.26	14	1
1:A:4:VAL:HG13	1:A:4:VAL:O	0.50	2.07	15	6
1:A:335:TYR:HB2	1:A:344:ALA:O	0.50	2.06	5	1
1:A:82:ALA:HB3	1:A:116:VAL:CG2	0.49	2.29	2	1
1:A:89:VAL:HG13	1:A:112:THR:O	0.49	2.07	14	2
1:A:351:LEU:HD11	1:A:366:PHE:HD1	0.49	1.65	1	1
1:A:335:TYR:CE2	1:A:345:LEU:HD12	0.49	2.42	6	2
1:A:335:TYR:HB2	1:A:345:LEU:HA	0.49	1.83	1	1
1:A:29:HIS:CE1	1:A:107:PHE:CE1	0.49	3.00	3	1
1:A:47:HIS:CD2	1:A:77:LEU:HD13	0.49	2.41	6	1
1:A:351:LEU:HD13	1:A:373:LEU:HD21	0.49	1.81	1	1
1:A:34:TRP:O	1:A:46:ILE:HD13	0.49	2.07	2	2
1:A:362:PHE:HB3	1:A:377:ILE:HD13	0.49	1.84	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ILE:CD1	1:A:60:ILE:O	0.49	2.60	2	2
1:A:45:LEU:HD21	1:A:48:TYR:CD2	0.49	2.42	8	1
1:A:306:SER:N	1:A:307:PRO:HD2	0.49	2.23	7	3
1:A:47:HIS:CD2	1:A:75:PHE:CZ	0.49	3.00	15	1
1:A:60:ILE:N	1:A:60:ILE:CD1	0.49	2.75	4	2
1:A:48:TYR:CG	1:A:48:TYR:O	0.49	2.66	5	2
1:A:329:PHE:CE1	1:A:332:PHE:CZ	0.49	3.01	7	2
1:A:114:LEU:HD12	1:A:114:LEU:C	0.49	2.28	15	2
1:A:310:LEU:HD23	1:A:311:THR:H	0.49	1.67	13	1
1:A:310:LEU:HD12	1:A:311:THR:N	0.49	2.23	14	1
1:A:312:VAL:CG2	1:A:412:LEU:HD12	0.49	2.38	13	1
1:A:388:TYR:CD1	1:A:412:LEU:HD21	0.49	2.43	14	1
1:A:27:ASN:O	1:A:28:ASN:CB	0.49	2.61	7	9
1:A:383:GLY:H	1:A:414:VAL:HG21	0.49	1.68	13	1
1:A:345:LEU:O	1:A:346:LEU:HD13	0.48	2.07	3	1
1:A:347:ILE:HD12	1:A:362:PHE:HZ	0.48	1.68	8	2
1:A:55:THR:O	1:A:56:GLU:CG	0.48	2.61	3	2
1:A:19:VAL:CG1	1:A:114:LEU:HD21	0.48	2.39	9	2
1:A:87:THR:HB	1:A:115:THR:HA	0.48	1.83	11	1
1:A:302:GLN:CD	1:A:405:THR:HG21	0.48	2.28	12	1
1:A:389:PHE:CE2	1:A:406:PHE:CE2	0.48	3.01	13	1
1:A:351:LEU:CD2	1:A:366:PHE:CD1	0.48	2.97	3	1
1:A:312:VAL:HG12	1:A:313:TRP:N	0.48	2.24	9	3
1:A:303:VAL:HG13	1:A:407:GLY:N	0.48	2.23	5	1
1:A:116(A):LEU:N	1:A:116(A):LEU:HD13	0.48	2.24	3	1
1:A:335:TYR:HB3	1:A:345:LEU:HD12	0.48	1.85	1	1
1:A:3:ALA:O	1:A:5:THR:CG2	0.48	2.60	14	3
1:A:43:LEU:HD23	1:A:44:ARG:N	0.48	2.24	4	1
1:A:105:GLU:HB2	1:A:345:LEU:HD22	0.48	1.85	5	1
1:A:320:LEU:HD11	1:A:388:TYR:CD1	0.48	2.44	15	1
1:A:319:ILE:C	1:A:319:ILE:HD12	0.48	2.28	7	1
1:A:47:HIS:NE2	1:A:67:ALA:HB2	0.48	2.24	12	1
1:A:373:LEU:HD12	1:A:373:LEU:N	0.48	2.24	6	1
1:A:412:LEU:HD12	1:A:412:LEU:C	0.48	2.29	8	2
1:A:93:ALA:HB2	1:A:108:PHE:CD2	0.47	2.44	5	1
1:A:35:TYR:CD1	1:A:36:ARG:N	0.47	2.82	4	1
1:A:82:ALA:CB	1:A:116:VAL:HG11	0.47	2.39	11	1
1:A:47:HIS:CE1	1:A:67:ALA:CB	0.47	2.97	14	1
1:A:65:TYR:CD1	1:A:65:TYR:N	0.47	2.82	9	6
1:A:335:TYR:CG	1:A:336:ARG:N	0.47	2.82	13	1
1:A:45:LEU:HD23	1:A:58:GLY:HA2	0.47	1.86	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:HIS:CE1	1:A:107:PHE:CD1	0.47	3.02	7	1
1:A:3:ALA:HB2	1:A:26:THR:HG22	0.47	1.85	9	1
1:A:105:GLU:CG	1:A:107:PHE:CZ	0.47	2.98	12	2
1:A:79:LEU:HD11	1:A:114:LEU:CD2	0.47	2.39	14	1
1:A:332:PHE:CE2	1:A:392:ALA:CB	0.47	2.98	12	4
1:A:311:THR:HG23	1:A:413:ALA:O	0.47	2.09	4	1
1:A:377:ILE:HG22	1:A:377:ILE:O	0.47	2.09	12	2
1:A:3:ALA:HB2	1:A:26:THR:CG2	0.47	2.39	9	1
1:A:350:SER:O	1:A:351:LEU:HG	0.47	2.10	4	1
1:A:51:GLY:O	1:A:52:ALA:HB3	0.47	2.09	11	2
1:A:15:THR:HG23	1:A:84:PRO:HG3	0.47	1.86	11	1
1:A:87:THR:OG1	1:A:114:LEU:O	0.47	2.24	11	1
1:A:90:TYR:CD1	1:A:90:TYR:N	0.47	2.83	11	1
1:A:105:GLU:HA	1:A:345:LEU:HD23	0.47	1.86	12	1
1:A:387:THR:HG22	1:A:411:ARG:HA	0.47	1.87	15	1
1:A:47:HIS:CD2	1:A:67:ALA:CB	0.47	2.97	9	1
1:A:312:VAL:HG22	1:A:318:THR:CG2	0.47	2.39	12	1
1:A:351:LEU:HD11	1:A:366:PHE:CE1	0.47	2.45	14	1
1:A:89:VAL:HG12	1:A:91:PHE:CD1	0.47	2.45	5	3
1:A:331:TYR:CZ	1:A:393:THR:CG2	0.46	2.98	1	2
1:A:338:PHE:HE1	1:A:346:LEU:HD21	0.46	1.67	1	1
1:A:375:LEU:C	1:A:375:LEU:HD23	0.46	2.29	15	10
1:A:33:TYR:N	1:A:33:TYR:CD1	0.46	2.83	9	5
1:A:50:TYR:CD2	1:A:51:GLY:N	0.46	2.84	11	2
1:A:41:HIS:CD2	1:A:42:GLY:N	0.46	2.83	10	1
1:A:311:THR:HG22	1:A:313:TRP:H	0.46	1.70	12	1
1:A:35:TYR:CE1	1:A:45:LEU:CD1	0.46	2.98	2	4
1:A:114:LEU:HD12	1:A:115:THR:O	0.46	2.09	11	1
1:A:82:ALA:HB3	1:A:116:VAL:CG1	0.46	2.35	3	2
1:A:33:TYR:CE1	1:A:404:LEU:HD12	0.46	2.46	4	1
1:A:48:TYR:N	1:A:48:TYR:CD1	0.46	2.84	5	4
1:A:83:THR:HG22	1:A:86:GLN:CG	0.46	2.36	6	1
1:A:362:PHE:CD1	1:A:375:LEU:CD1	0.46	2.98	15	4
1:A:335:TYR:O	1:A:336:ARG:CB	0.46	2.64	1	2
1:A:42:GLY:CA	1:A:408:ALA:HA	0.46	2.40	2	1
1:A:35:TYR:CZ	1:A:45:LEU:CD1	0.46	2.99	5	5
1:A:365:PHE:CE1	1:A:376:HIS:CD2	0.46	3.03	12	1
1:A:35:TYR:CZ	1:A:45:LEU:HD13	0.46	2.45	1	1
1:A:47:HIS:CE1	1:A:77:LEU:HD13	0.46	2.46	1	1
1:A:345:LEU:C	1:A:345:LEU:HD23	0.46	2.31	11	1
1:A:20:THR:HA	1:A:78:ILE:HG22	0.46	1.87	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:306:SER:CB	1:A:307:PRO:HD3	0.46	2.41	11	2
1:A:60:ILE:CG1	1:A:60:ILE:O	0.46	2.64	12	2
1:A:78:ILE:C	1:A:79:LEU:HD12	0.46	2.31	3	2
1:A:93:ALA:HB1	1:A:106:GLN:OE1	0.46	2.11	4	1
1:A:349:ILE:N	1:A:349:ILE:CD1	0.46	2.79	10	6
1:A:83:THR:OG1	1:A:84:PRO:HD2	0.46	2.11	9	2
1:A:331:TYR:CE1	1:A:393:THR:CG2	0.46	2.99	13	1
1:A:393:THR:HG22	1:A:404:LEU:HG	0.46	1.87	14	1
1:A:89:VAL:CG1	1:A:91:PHE:CE2	0.46	2.98	1	2
1:A:21:LEU:HD11	1:A:90:TYR:CG	0.46	2.45	13	2
1:A:4:VAL:HA	1:A:24:ASN:O	0.46	2.11	9	2
1:A:388:TYR:CD1	1:A:388:TYR:N	0.45	2.84	5	2
1:A:320:LEU:CD2	1:A:388:TYR:CG	0.45	2.99	12	1
1:A:336:ARG:CB	1:A:346:LEU:HD21	0.45	2.41	12	2
1:A:65:TYR:HB2	1:A:78:ILE:O	0.45	2.11	14	1
1:A:93:ALA:CB	1:A:108:PHE:CD1	0.45	2.99	14	1
1:A:349:ILE:HG21	1:A:364:ILE:HD13	0.45	1.86	3	1
1:A:21:LEU:CD1	1:A:90:TYR:CG	0.45	2.99	8	3
1:A:43:LEU:HD23	1:A:389:PHE:CE2	0.45	2.46	9	1
1:A:69:ARG:CD	1:A:75:PHE:CD2	0.45	3.00	3	1
1:A:384:ASP:O	1:A:385:SER:CB	0.45	2.62	13	6
1:A:401:PHE:CD1	1:A:401:PHE:N	0.45	2.84	13	1
1:A:338:PHE:N	1:A:339:PRO:CD	0.45	2.79	1	1
1:A:332:PHE:CE1	1:A:392:ALA:CB	0.45	3.00	6	3
1:A:331:TYR:CD1	1:A:331:TYR:N	0.45	2.85	6	2
1:A:47:HIS:CE1	1:A:67:ALA:HB3	0.45	2.46	14	1
1:A:47:HIS:NE2	1:A:65:TYR:CE1	0.45	2.84	14	1
1:A:60:ILE:HG12	1:A:60:ILE:O	0.45	2.12	7	1
1:A:47:HIS:CD2	1:A:67:ALA:HB2	0.45	2.46	9	1
1:A:35:TYR:CD2	1:A:36:ARG:N	0.45	2.85	10	1
1:A:326:ASP:CB	1:A:329:PHE:CZ	0.45	2.99	11	1
1:A:31:ASN:ND2	1:A:33:TYR:CZ	0.45	2.85	2	1
1:A:332:PHE:N	1:A:332:PHE:CD1	0.45	2.84	4	3
1:A:41:HIS:CD2	1:A:41:HIS:N	0.45	2.84	11	3
1:A:389:PHE:CE2	1:A:406:PHE:CZ	0.45	3.04	13	1
1:A:319:ILE:C	1:A:320:LEU:HD12	0.45	2.32	7	1
1:A:116(A):LEU:C	1:A:116(A):LEU:HD23	0.45	2.32	4	2
1:A:375:LEU:HD23	1:A:375:LEU:O	0.45	2.12	2	3
1:A:50:TYR:CG	1:A:51:GLY:N	0.45	2.84	5	1
1:A:25:GLN:C	1:A:26:THR:HG23	0.45	2.32	14	1
1:A:17:GLY:O	1:A:18:LYS:CB	0.45	2.64	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:GLN:HE22	1:A:21:LEU:HD22	0.45	1.71	1	1
1:A:329:PHE:CD1	1:A:329:PHE:O	0.45	2.70	14	7
1:A:303:VAL:HG21	1:A:391:ALA:HA	0.45	1.89	2	2
1:A:34:TRP:CE3	1:A:91:PHE:O	0.45	2.70	6	3
1:A:41:HIS:C	1:A:41:HIS:CD2	0.45	2.90	6	1
1:A:332:PHE:CD1	1:A:392:ALA:CB	0.44	3.00	2	1
1:A:36:ARG:NE	1:A:90:TYR:CE2	0.44	2.85	5	1
1:A:329:PHE:CD1	1:A:392:ALA:HB1	0.44	2.47	5	1
1:A:35:TYR:HA	1:A:46:ILE:HD11	0.44	1.89	11	1
1:A:13:ALA:CB	1:A:116:VAL:HG22	0.44	2.39	13	1
1:A:353:SER:O	1:A:354:ASN:CB	0.44	2.63	1	1
1:A:391:ALA:HA	1:A:405:THR:O	0.44	2.13	7	1
1:A:35:TYR:CD2	1:A:43:LEU:CD1	0.44	3.01	10	1
1:A:13:ALA:HB3	1:A:116:VAL:CG2	0.44	2.42	14	1
1:A:15:THR:N	1:A:116(A):LEU:O	0.44	2.51	2	1
1:A:351:LEU:CD2	1:A:366:PHE:CE1	0.44	2.99	8	1
1:A:389:PHE:CD1	1:A:389:PHE:C	0.44	2.91	13	1
1:A:106:GLN:OE1	1:A:335:TYR:CE1	0.44	2.71	14	1
1:A:52:ALA:HB2	1:A:72:GLN:CB	0.44	2.43	1	1
1:A:50:TYR:CD1	1:A:51:GLY:N	0.44	2.86	15	2
1:A:367:ASN:O	1:A:371:LYS:N	0.44	2.51	2	2
1:A:324:TYR:CD1	1:A:324:TYR:N	0.44	2.85	13	7
1:A:312:VAL:HG22	1:A:313:TRP:N	0.44	2.28	10	4
1:A:318:THR:O	1:A:377:ILE:HG22	0.44	2.12	5	1
1:A:342:SER:N	1:A:343:PRO:HD3	0.44	2.27	12	2
1:A:336:ARG:HD3	1:A:346:LEU:HD21	0.44	1.88	14	1
1:A:39:THR:HG22	1:A:40:GLY:H	0.44	1.73	7	2
1:A:33:TYR:CD1	1:A:33:TYR:N	0.44	2.86	14	1
1:A:47:HIS:CE1	1:A:55:THR:HG22	0.44	2.48	15	1
1:A:408:ALA:O	1:A:409:GLY:C	0.44	2.54	10	2
1:A:83:THR:O	1:A:85:SER:N	0.44	2.46	6	3
1:A:77:LEU:C	1:A:77:LEU:CD1	0.44	2.81	15	1
1:A:48:TYR:CD2	1:A:48:TYR:O	0.44	2.71	7	3
1:A:345:LEU:C	1:A:346:LEU:HD22	0.43	2.33	3	1
1:A:91:PHE:CD1	1:A:91:PHE:C	0.43	2.91	4	1
1:A:6:GLN:HA	1:A:22:SER:O	0.43	2.13	11	4
1:A:29:HIS:NE2	1:A:107:PHE:CE1	0.43	2.86	8	1
1:A:337:GLN:NE2	1:A:389:PHE:CZ	0.43	2.86	8	1
1:A:385:SER:CA	1:A:414:VAL:HG23	0.43	2.43	8	1
1:A:44:ARG:HD2	1:A:60:ILE:HD11	0.43	1.89	9	1
1:A:338:PHE:N	1:A:338:PHE:CD1	0.43	2.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TYR:O	1:A:48:TYR:CD1	0.43	2.71	14	1
1:A:302:GLN:CG	1:A:303:VAL:N	0.43	2.81	14	1
1:A:311:THR:O	1:A:311:THR:HG23	0.43	2.13	1	1
1:A:35:TYR:HB2	1:A:91:PHE:CZ	0.43	2.49	2	2
1:A:116(A):LEU:HD22	1:A:116(A):LEU:O	0.43	2.12	3	1
1:A:363:THR:O	1:A:375:LEU:HA	0.43	2.13	15	3
1:A:389:PHE:CD1	1:A:389:PHE:O	0.43	2.71	5	2
1:A:93:ALA:CB	1:A:108:PHE:CE1	0.43	3.00	11	2
1:A:329:PHE:CD1	1:A:329:PHE:N	0.43	2.84	6	1
1:A:332:PHE:HD1	1:A:392:ALA:HB2	0.43	1.70	7	1
1:A:312:VAL:HG12	1:A:314:GLU:H	0.43	1.73	13	1
1:A:47:HIS:NE2	1:A:65:TYR:CE2	0.43	2.85	3	1
1:A:387:THR:HG22	1:A:411:ARG:CG	0.43	2.43	10	1
1:A:35:TYR:CB	1:A:91:PHE:CZ	0.43	3.01	15	1
1:A:335:TYR:CE1	1:A:345:LEU:HD13	0.43	2.49	3	1
1:A:33:TYR:CE2	1:A:106:GLN:NE2	0.43	2.87	12	1
1:A:43:LEU:O	1:A:406:PHE:CE2	0.43	2.71	12	1
1:A:25:GLN:HG2	1:A:29:HIS:CE1	0.43	2.49	13	1
1:A:93:ALA:HB2	1:A:108:PHE:CZ	0.43	2.47	1	1
1:A:392:ALA:O	1:A:405:THR:N	0.43	2.52	7	1
1:A:320:LEU:N	1:A:320:LEU:HD12	0.43	2.28	10	2
1:A:21:LEU:HD13	1:A:90:TYR:CB	0.43	2.44	3	1
1:A:77:LEU:C	1:A:78:ILE:HG23	0.43	2.35	6	2
1:A:44:ARG:HD3	1:A:60:ILE:HD11	0.43	1.91	12	1
1:A:43:LEU:HD13	1:A:406:PHE:CE2	0.43	2.49	13	1
1:A:313:TRP:O	1:A:314:GLU:O	0.43	2.36	13	1
1:A:12:VAL:HG12	1:A:13:ALA:N	0.42	2.29	1	6
1:A:381:GLN:N	1:A:382:PRO:HD3	0.42	2.29	8	1
1:A:115:THR:HG22	1:A:116(A):LEU:HD23	0.42	1.91	11	1
1:A:342:SER:N	1:A:343:PRO:CD	0.42	2.82	12	2
1:A:332:PHE:CD2	1:A:391:ALA:O	0.42	2.72	4	1
1:A:381:GLN:N	1:A:382:PRO:HD2	0.42	2.30	11	3
1:A:29:HIS:O	1:A:29:HIS:CD2	0.42	2.72	13	1
1:A:86:GLN:O	1:A:87:THR:O	0.42	2.37	15	1
1:A:391:ALA:HB2	1:A:406:PHE:CG	0.42	2.48	2	2
1:A:331:TYR:HB2	1:A:393:THR:HG23	0.42	1.91	3	1
1:A:319:ILE:HG22	1:A:376:HIS:ND1	0.42	2.29	7	1
1:A:306:SER:CB	1:A:307:PRO:CD	0.42	2.97	8	2
1:A:47:HIS:ND1	1:A:67:ALA:HB2	0.42	2.29	11	1
1:A:383:GLY:CA	1:A:414:VAL:HG21	0.42	2.43	13	1
1:A:338:PHE:HB2	1:A:339:PRO:HD3	0.42	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:LEU:C	1:A:320:LEU:HD23	0.42	2.35	3	1
1:A:351:LEU:HD21	1:A:366:PHE:CD1	0.42	2.49	12	2
1:A:41:HIS:CG	1:A:408:ALA:HB1	0.42	2.49	4	1
1:A:392:ALA:O	1:A:404:LEU:HD23	0.42	2.15	5	1
1:A:43:LEU:HD12	1:A:406:PHE:CD2	0.42	2.49	11	2
1:A:49:SER:CB	1:A:69:ARG:NH1	0.42	2.83	13	1
1:A:306:SER:O	1:A:308:GLN:N	0.42	2.51	2	3
1:A:55:THR:HG23	1:A:56:GLU:HG2	0.42	1.92	3	1
1:A:365:PHE:CD1	1:A:365:PHE:O	0.42	2.73	8	1
1:A:401:PHE:O	1:A:401:PHE:CG	0.42	2.73	9	1
1:A:303:VAL:CG1	1:A:407:GLY:CA	0.42	2.96	13	1
1:A:48:TYR:CD1	1:A:48:TYR:N	0.42	2.87	15	1
1:A:338:PHE:CZ	1:A:346:LEU:HD21	0.42	2.48	1	1
1:A:41:HIS:CG	1:A:44:ARG:NH1	0.42	2.88	7	1
1:A:48:TYR:CD2	1:A:402:ASN:CB	0.42	3.03	7	1
1:A:336:ARG:HG3	1:A:346:LEU:HD11	0.42	1.91	8	1
1:A:93:ALA:CA	1:A:108:PHE:HB3	0.42	2.44	12	1
1:A:46:ILE:O	1:A:58:GLY:N	0.42	2.53	2	4
1:A:60:ILE:HD12	1:A:60:ILE:C	0.42	2.34	11	2
1:A:89:VAL:HG12	1:A:91:PHE:CE1	0.42	2.49	5	1
1:A:18:LYS:C	1:A:19:VAL:CG2	0.42	2.87	14	1
1:A:78:ILE:HG23	1:A:79:LEU:N	0.42	2.29	14	1
1:A:338:PHE:CB	1:A:339:PRO:HD3	0.42	2.45	1	1
1:A:47:HIS:NE2	1:A:67:ALA:CB	0.42	2.82	2	2
1:A:91:PHE:CD1	1:A:91:PHE:N	0.42	2.88	2	1
1:A:336:ARG:CD	1:A:388:TYR:CE1	0.42	3.02	3	1
1:A:337:GLN:NE2	1:A:389:PHE:CE1	0.42	2.88	8	1
1:A:61:PRO:HB3	1:A:65:TYR:CE1	0.42	2.50	11	1
1:A:322:CYS:HB3	1:A:373:LEU:HD21	0.42	1.92	11	1
1:A:34:TRP:CE2	1:A:77:LEU:CD2	0.42	3.03	12	1
1:A:3:ALA:N	1:A:26:THR:CG2	0.42	2.83	1	3
1:A:38:ASP:O	1:A:39:THR:O	0.42	2.38	1	1
1:A:41:HIS:O	1:A:43:LEU:N	0.42	2.53	9	2
1:A:362:PHE:CE1	1:A:377:ILE:CD1	0.42	3.02	11	1
1:A:320:LEU:HD22	1:A:375:LEU:HB3	0.42	1.92	3	1
1:A:319:ILE:HD12	1:A:319:ILE:N	0.42	2.30	8	1
1:A:381:GLN:CB	1:A:382:PRO:HD2	0.42	2.45	13	1
1:A:41:HIS:O	1:A:389:PHE:CZ	0.42	2.73	15	1
1:A:346:LEU:C	1:A:347:ILE:HG23	0.41	2.36	1	2
1:A:48:TYR:O	1:A:48:TYR:CG	0.41	2.73	13	3
1:A:305:GLN:NE2	1:A:409:GLY:CA	0.41	2.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:335:TYR:CG	1:A:345:LEU:HA	0.41	2.49	5	1
1:A:87:THR:CG2	1:A:114:LEU:CD1	0.41	2.98	6	2
1:A:93:ALA:HB1	1:A:106:GLN:HG3	0.41	1.91	9	1
1:A:338:PHE:CD1	1:A:338:PHE:N	0.41	2.88	10	1
1:A:375:LEU:HG	1:A:376:HIS:N	0.41	2.31	13	2
1:A:67:ALA:CB	1:A:77:LEU:HD22	0.41	2.45	14	1
1:A:375:LEU:HD23	1:A:375:LEU:C	0.41	2.36	2	3
1:A:29:HIS:NE2	1:A:107:PHE:CD1	0.41	2.88	3	1
1:A:336:ARG:HD3	1:A:388:TYR:CE1	0.41	2.50	3	1
1:A:346:LEU:CB	1:A:347:ILE:HD13	0.41	2.42	6	1
1:A:45:LEU:CA	1:A:46:ILE:HD13	0.41	2.44	11	1
1:A:106:GLN:OE1	1:A:108:PHE:CZ	0.41	2.73	1	1
1:A:336:ARG:HG2	1:A:389:PHE:CD1	0.41	2.50	1	1
1:A:29:HIS:CD2	1:A:95:GLY:O	0.41	2.74	5	1
1:A:47:HIS:HE1	1:A:77:LEU:HD13	0.41	1.76	1	1
1:A:335:TYR:CD1	1:A:335:TYR:C	0.41	2.94	1	1
1:A:19:VAL:O	1:A:78:ILE:HB	0.41	2.15	2	1
1:A:48:TYR:O	1:A:48:TYR:CD2	0.41	2.73	5	2
1:A:46:ILE:O	1:A:47:HIS:ND1	0.41	2.54	9	1
1:A:337:GLN:OE1	1:A:389:PHE:CZ	0.41	2.74	9	1
1:A:29:HIS:O	1:A:29:HIS:CG	0.41	2.73	14	1
1:A:389:PHE:CE2	1:A:408:ALA:O	0.41	2.74	14	1
1:A:334:TRP:CD1	1:A:334:TRP:C	0.41	2.92	3	1
1:A:35:TYR:HE2	1:A:43:LEU:HD22	0.41	1.69	9	1
1:A:333:PRO:O	1:A:335:TYR:N	0.41	2.54	6	1
1:A:34:TRP:CE2	1:A:77:LEU:HD21	0.41	2.50	12	1
1:A:43:LEU:O	1:A:406:PHE:CZ	0.41	2.74	15	1
1:A:65:TYR:CZ	1:A:79:LEU:CD1	0.41	3.04	1	1
1:A:87:THR:CB	1:A:115:THR:HA	0.41	2.45	3	1
1:A:331:TYR:CB	1:A:393:THR:CG2	0.41	2.99	3	1
1:A:331:TYR:CD1	1:A:349:ILE:O	0.41	2.74	3	1
1:A:41:HIS:CD2	1:A:43:LEU:O	0.41	2.74	13	2
1:A:412:LEU:N	1:A:412:LEU:CD2	0.41	2.83	7	1
1:A:34:TRP:CB	1:A:47:HIS:CB	0.41	2.99	12	1
1:A:5:THR:O	1:A:23:CYS:HA	0.41	2.15	9	2
1:A:332:PHE:CD1	1:A:332:PHE:N	0.41	2.88	14	3
1:A:61:PRO:O	1:A:62:ASP:O	0.41	2.39	3	1
1:A:4:VAL:C	1:A:5:THR:CG2	0.41	2.89	5	2
1:A:31:ASN:OD1	1:A:33:TYR:CZ	0.41	2.74	5	1
1:A:43:LEU:O	1:A:406:PHE:CE1	0.41	2.74	7	1
1:A:12:VAL:CG1	1:A:13:ALA:N	0.41	2.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:HIS:CE1	1:A:44:ARG:HG2	0.41	2.51	1	1
1:A:68:SER:O	1:A:75:PHE:CD1	0.41	2.74	2	2
1:A:34:TRP:HB2	1:A:47:HIS:O	0.41	2.16	3	3
1:A:3:ALA:CA	1:A:26:THR:CG2	0.41	2.98	4	1
1:A:25:GLN:NE2	1:A:29:HIS:NE2	0.41	2.69	4	1
1:A:89:VAL:HA	1:A:112:THR:O	0.41	2.15	15	2
1:A:375:LEU:HD12	1:A:375:LEU:C	0.41	2.36	7	1
1:A:412:LEU:N	1:A:412:LEU:HD22	0.41	2.30	7	1
1:A:19:VAL:CG2	1:A:79:LEU:HB2	0.41	2.46	9	1
1:A:385:SER:OG	1:A:414:VAL:HG23	0.41	2.16	1	1
1:A:4:VAL:CG1	1:A:107:PHE:O	0.41	2.69	4	1
1:A:35:TYR:CD2	1:A:91:PHE:CD1	0.41	3.08	4	1
1:A:336:ARG:HG3	1:A:337:GLN:N	0.40	2.30	1	1
1:A:29:HIS:CD2	1:A:94:SER:OG	0.40	2.73	3	1
1:A:334:TRP:CZ3	1:A:388:TYR:HB3	0.40	2.50	3	1
1:A:60:ILE:O	1:A:60:ILE:HG12	0.40	2.15	4	1
1:A:63:GLY:O	1:A:79:LEU:HD13	0.40	2.16	4	1
1:A:4:VAL:O	1:A:4:VAL:HG13	0.40	2.15	1	1
1:A:336:ARG:O	1:A:343:PRO:HB3	0.40	2.16	5	1
1:A:389:PHE:CE2	1:A:391:ALA:CB	0.40	3.04	5	1
1:A:329:PHE:CD1	1:A:332:PHE:CZ	0.40	3.09	7	1
1:A:362:PHE:O	1:A:362:PHE:CD1	0.40	2.74	7	1
1:A:381:GLN:N	1:A:382:PRO:CD	0.40	2.84	15	2
1:A:365:PHE:N	1:A:374:SER:O	0.40	2.54	12	1
1:A:351:LEU:CG	1:A:366:PHE:CE1	0.40	3.04	14	1
1:A:27:ASN:OD1	1:A:29:HIS:CE1	0.40	2.74	5	1
1:A:52:ALA:HB2	1:A:72:GLN:HG3	0.40	1.91	10	1
1:A:313:TRP:CD1	1:A:316:GLU:OE2	0.40	2.74	10	1
1:A:29:HIS:CD2	1:A:94:SER:O	0.40	2.75	12	1
1:A:25:GLN:OE1	1:A:29:HIS:CG	0.40	2.74	14	1
1:A:21:LEU:CD1	1:A:90:TYR:CD2	0.40	3.04	15	1
1:A:105:GLU:O	1:A:107:PHE:CE2	0.40	2.75	4	1
1:A:365:PHE:CD1	1:A:365:PHE:C	0.40	2.93	5	1
1:A:35:TYR:CE1	1:A:91:PHE:CB	0.40	3.05	9	1
1:A:33:TYR:CE1	1:A:106:GLN:NE2	0.40	2.89	10	1
1:A:43:LEU:O	1:A:406:PHE:CD2	0.40	2.75	12	1
1:A:49:SER:CB	1:A:75:PHE:CZ	0.40	3.04	12	1
1:A:19:VAL:HB	1:A:79:LEU:HB2	0.40	1.92	13	1
1:A:63:GLY:O	1:A:79:LEU:CD1	0.40	2.70	13	1
1:A:362:PHE:CD1	1:A:375:LEU:HD12	0.40	2.52	5	1
1:A:401:PHE:O	1:A:401:PHE:CD1	0.40	2.75	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:TYR:CD1	1:A:93:ALA:O	0.40	2.74	10	1
1:A:351:LEU:HD23	1:A:366:PHE:CE1	0.40	2.52	11	1

6.3 Torsion angles [\(i\)](#)

6.3.1 Protein backbone [\(i\)](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/249 (86%)	155±4 (73±2%)	41±3 (19±2%)	18±3 (8±2%)	2	13
All	All	3210/3735 (86%)	2332 (73%)	610 (19%)	268 (8%)	2	13

All 60 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	85	SER	15
1	A	88	SER	15
1	A	349	ILE	15
1	A	26	THR	14
1	A	347	ILE	14
1	A	314	GLU	11
1	A	87	THR	10
1	A	385	SER	10
1	A	408	ALA	10
1	A	309	SER	10
1	A	308	GLN	9
1	A	350	SER	9
1	A	58	GLY	8
1	A	382	PRO	7
1	A	61	PRO	7
1	A	307	PRO	6
1	A	381	GLN	6
1	A	52	ALA	5
1	A	409	GLY	5
1	A	334	TRP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	8	PRO	5
1	A	39	THR	4
1	A	110	PRO	4
1	A	340	GLY	4
1	A	42	GLY	4
1	A	116(A)	LEU	3
1	A	62	ASP	3
1	A	43	LEU	3
1	A	328	THR	3
1	A	333	PRO	2
1	A	336	ARG	2
1	A	339	PRO	2
1	A	301	GLN	2
1	A	316	GLU	2
1	A	330	ASP	2
1	A	301(A)	GLN	2
1	A	404	LEU	2
1	A	9	ARG	2
1	A	56	GLU	2
1	A	341	LYS	2
1	A	400	SER	2
1	A	377	ILE	2
1	A	55	THR	1
1	A	7	SER	1
1	A	95	GLY	1
1	A	41	HIS	1
1	A	383	GLY	1
1	A	4	VAL	1
1	A	63	GLY	1
1	A	402	ASN	1
1	A	54	SER	1
1	A	361	ARG	1
1	A	344	ALA	1
1	A	401	PHE	1
1	A	414	VAL	1
1	A	306	SER	1
1	A	403	LYS	1
1	A	18	LYS	1
1	A	79	LEU	1
1	A	399	GLY	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/202 (91%)	139±7 (76±4%)	44±7 (24±4%)	2	26
All	All	2745/3030 (91%)	2078 (76%)	667 (24%)	2	26

All 128 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	46	ILE	15
1	A	88	SER	15
1	A	347	ILE	15
1	A	364	ILE	15
1	A	34	TRP	14
1	A	78	ILE	14
1	A	87	THR	14
1	A	375	LEU	13
1	A	113	ARG	12
1	A	114	LEU	12
1	A	116(A)	LEU	12
1	A	18	LYS	11
1	A	39	THR	11
1	A	335	TYR	10
1	A	44	ARG	9
1	A	306	SER	9
1	A	356	LYS	9
1	A	403	LYS	9
1	A	36	ARG	9
1	A	66	LYS	8
1	A	79	LEU	8
1	A	304	ARG	8
1	A	323	SER	8
1	A	341	LYS	8
1	A	351	LEU	8
1	A	9	ARG	8
1	A	85	SER	8
1	A	6	GLN	7
1	A	60	ILE	7

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Mol	Chain	Res	Type	Models (Total)
1	A	105	GLU	7
1	A	301	GLN	7
1	A	314	GLU	7
1	A	355	LYS	7
1	A	71	SER	7
1	A	336	ARG	7
1	A	7	SER	7
1	A	373	LEU	7
1	A	54	SER	6
1	A	57	LYS	6
1	A	72	GLN	6
1	A	81	LEU	6
1	A	15	THR	6
1	A	32	MET	6
1	A	77	LEU	6
1	A	305	GLN	6
1	A	349	ILE	6
1	A	337	GLN	6
1	A	48	TYR	5
1	A	86	GLN	5
1	A	371	LYS	5
1	A	372	LYS	5
1	A	62	ASP	5
1	A	301(A)	GLN	5
1	A	308	GLN	5
1	A	327	SER	5
1	A	361	ARG	5
1	A	75	PHE	5
1	A	313	TRP	5
1	A	365	PHE	5
1	A	381	GLN	5
1	A	411	ARG	5
1	A	326	ASP	5
1	A	11	LYS	5
1	A	106	GLN	5
1	A	302	GLN	5
1	A	385	SER	5
1	A	28	ASN	4
1	A	74	ASN	4
1	A	342	SER	4
1	A	357	GLU	4
1	A	367	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	43	LEU	4
1	A	45	LEU	4
1	A	47	HIS	4
1	A	55	THR	4
1	A	412	LEU	4
1	A	41	HIS	4
1	A	59	ASP	4
1	A	404	LEU	4
1	A	410	THR	4
1	A	380	SER	4
1	A	38	ASP	3
1	A	56	GLU	3
1	A	310	LEU	3
1	A	402	ASN	3
1	A	25	GLN	3
1	A	320	LEU	3
1	A	334	TRP	3
1	A	35	TYR	3
1	A	318	THR	3
1	A	374	SER	3
1	A	384	ASP	3
1	A	69	ARG	3
1	A	316	GLU	3
1	A	358	ASP	3
1	A	368	LYS	3
1	A	369	ARG	3
1	A	379	ASP	2
1	A	31	ASN	2
1	A	353	SER	2
1	A	390	CYS	2
1	A	37	GLN	2
1	A	366	PHE	2
1	A	389	PHE	2
1	A	377	ILE	2
1	A	400	SER	2
1	A	49	SER	2
1	A	27	ASN	2
1	A	338	PHE	1
1	A	30	ASN	1
1	A	68	SER	1
1	A	91	PHE	1
1	A	330	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	10	ASN	1
1	A	80	GLU	1
1	A	354	ASN	1
1	A	73	GLU	1
1	A	83	THR	1
1	A	325	GLU	1
1	A	94	SER	1
1	A	378	THR	1
1	A	24	ASN	1
1	A	370	GLU	1
1	A	309	SER	1
1	A	322	CYS	1
1	A	5	THR	1
1	A	321	ASN	1
1	A	401	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided