Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2022 – 03:51 PM EST

PDB ID	:	1F8H
Title	:	STRUCTURE OF THE SECOND EPS15 HOMOLOGY DOMAIN OF HUMAN EPS15 IN COMPLEX WITH PTGSSSTNPFR
Authors	:	De Beer, T.; Hoofnagle, A.N.; Enmon, J.L.; Bowers, R.C.; Yamabhai, M.; Kay, B.K.; Overduin, M.
Deposited on	:	2000-06-30

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 (i) symbol.

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

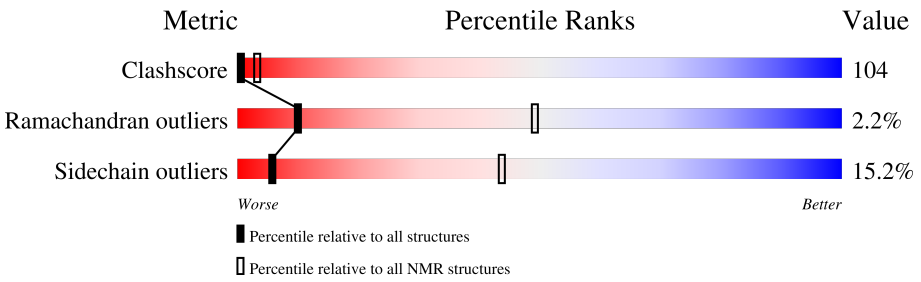
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	95	8% 69% 6% 16%
2	B	11	27% 9% 18% 45%

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 8 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	A:7-A:81, A:85-A:89, B:109-B:112 (84)	0.23	8

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

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

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

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1593 atoms, of which 799 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1494	484	752	118	136	4	0

- Molecule 2 is a protein called PTGSSSTNPFR.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	6	98	31	47	10	10	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	1	1	1

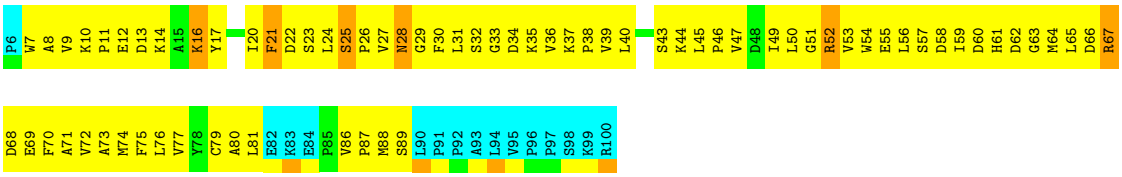
4 Residue-property plots (i)

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: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 8% 69% 6% 16%



• Molecule 2: PTGSSSTNPFR

Chain B: 27% 9% 18% 45%

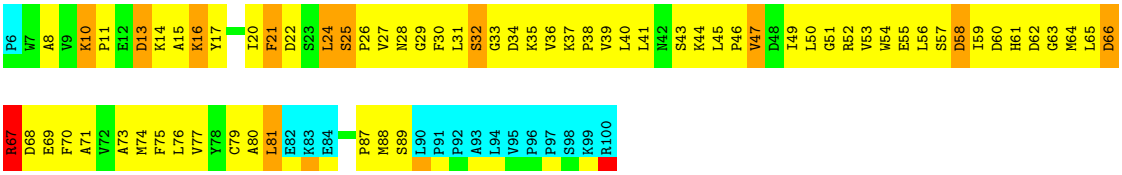
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 13% 59% 12% • 16%



• Molecule 2: PTGSSSTNPFR

Chain B: 27% 9% 18% 45%

PRO THR GLY SER SER S107 T108 N109 P110 F111 R112

4.2.2 Score per residue for model 2

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 12% 66% 5% • 16%

P6 W7 A8 V9 K10 P11 E12 D13 K16 Y17 D18 A19 I20 F21 D22 S23 L24 S25 P26 V27 N28 G29 F30 L31 S32 G33 D34 K35 V36 K37 P38 V39 L40 S43 K44 L45 P46 V47 D48 I49 L50 G51 R52 V53 W54 E55 L56 S57 D58 I59 D60 H61 D62 G63 M64 L65 D66 R67

D68 E69 F70 A71 V72 A73 M74 F75 L76 V77 Y78 C79 A80 L81 E82 K83 E84 P85 V86 P87 M88 S89 L90 P91 P92 A93 L94 V95 P96 P97 S98 K99 R100

- Molecule 2: PTGSSSTNPFR

Chain B: 36% 18% 45%

PRO THR GLY SER SER S107 T108 N109 P110 F111 R112

4.2.3 Score per residue for model 3

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 12% 63% 8% • 16%

P6 W7 A8 V9 K10 P11 E12 D13 K14 A15 K16 Y17 I20 F21 D22 S23 L24 S25 P26 V27 N28 G29 F30 L31 S32 G33 D34 K35 V36 K37 P38 V39 L40 L41 N42 S43 K44 L45 P46 V47 D48 I49 L50 G51 R52 V53 W54 E55 L56 S57 D58 I59 D60 H61 D62 G63 M64 L65 D66

R67 D68 E69 F70 A71 V72 A73 M74 F75 L76 V77 Y78 C79 A80 L81 E82 K83 E84 P87 M88 S89 L90 P91 P92 A93 L94 V95 P96 P97 S98 K99 R100

- Molecule 2: PTGSSSTNPFR

Chain B: 27% 9% 18% 45%

PRO THR GLY SER SER S107 T108 N109 P110 F111 R112

4.2.4 Score per residue for model 4

- Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 9% 67% 6% • 16%

P6 W7 A8 V9 K10 P11 E12 D13 K14 A15 K16 Y17 I20 F21 D22 S23 L24 S25 P26 V27 N28 G29 F30 L31 S32 G33 D34 K35 V36 K37 P38 V39 L40 L41 N42 S43 K44 L45 P46 V47 D48 I49 L50 G51 R52 V53 W54 E55 L56 S57 D58 I59 D60 H61 D62 G63 M64 L65 D66

R67 D68 E69 F70 A71 V72 A73 M74 F75 L76 V77 Y78 C79 A80 L81 E82 K83 E84 P85 V86 P87 M88 S89 L90 P91 P92 A93 L94 V95 P96 P97 S98 K99 R100

• Molecule 2: PTGSSSTNPFR

Chain B: 18% 18% 18% 45%

PRO THR GLY SER SER S107 T108 N109 P110 F111 R112

4.2.5 Score per residue for model 5

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 6% 69% 7% • 16%

P6 W7 A8 V9 K10 P11 E12 D13 K14 A15 K16 Y17 D18 A19 I20 F21 D22 S23 L24 S25 P26 V27 N28 G29 F30 L31 S32 G33 D34 K35 V36 K37 P38 V39 L40 S43 K44 L45 P46 V47 D48 I49 L50 G51 R52 V53 W54 E55 L56 S57 D58 I59 D60 H61 D62 G63 M64 L65 D66

R67 D68 E69 F70 A71 V72 A73 M74 F75 L76 V77 Y78 C79 A80 L81 E82 K83 E84 P85 V86 P87 M88 S89 L90 P91 P92 A93 L94 V95 P96 P97 S98 K99 R100

• Molecule 2: PTGSSSTNPFR

Chain B: 36% 18% 45%

PRO THR GLY SER SER S107 T108 N109 P110 F111 R112

4.2.6 Score per residue for model 6

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

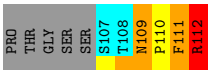
Chain A: 14% 60% 11% 16%

P6 W7 A8 V9 E12 D13 K14 A15 K16 Y17 I20 F21 D22 S23 L24 S25 P26 V27 N28 L31 S32 G33 D34 K35 V36 K37 P38 V39 L40 S43 K44 L45 P46 V47 D48 I49 L50 G51 R52 V53 W54 E55 L56 S57 D58 I59 D60 H61 D62 G63 M64 L65 D66 R67 D68 E69

F70 A71 V72 A73 M74 F75 L76 V77 Y78 C79 A80 L81 E82 K83 E84 P85 V86 P87 M88 S89 L90 P91 P92 A93 L94 V95 P96 P97 S98 K99 R100

• Molecule 2: PTGSSSTNPFR

Chain B: 9% 18% 9% 18% 45%



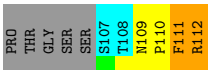
4.2.7 Score per residue for model 7

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:

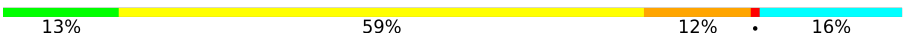
• Molecule 2: PTGSSSTNPFR

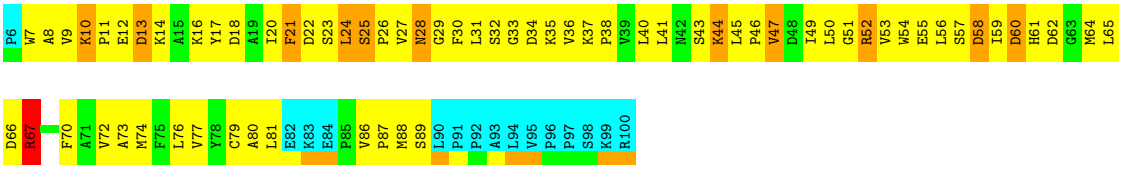
Chain B:



4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A: 



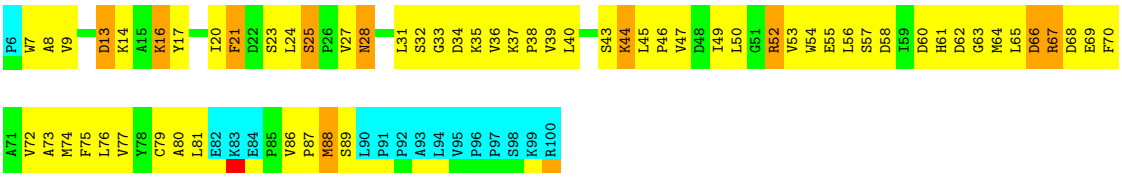
• Molecule 2: PTGSSSTNPFR

Chain B:

4.2.9 Score per residue for model 9

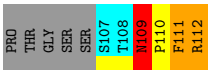
• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:



• Molecule 2: PTGSSSTNPFR

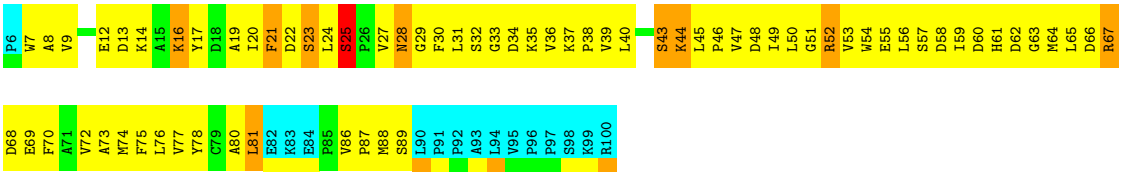
Chain B:



4.2.10 Score per residue for model 10

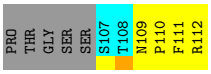
• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:



• Molecule 2: PTGSSSTNPFR

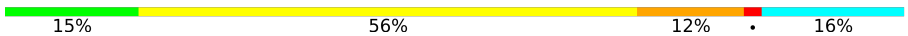
Chain B:



4.2.11 Score per residue for model 11

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:



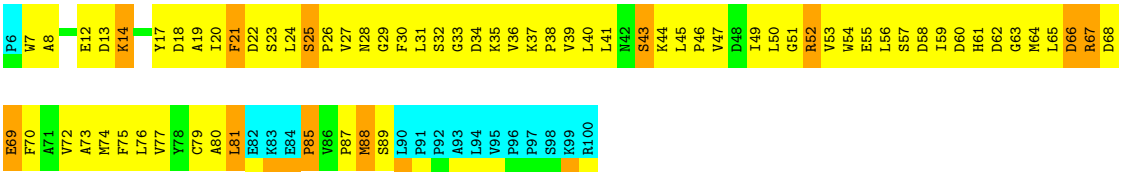
• Molecule 2: PTGSSSTNPFR

Chain B:

4.2.12 Score per residue for model 12

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:



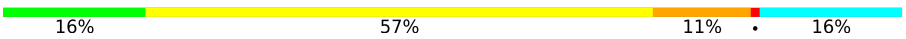
• Molecule 2: PTGSSSTNPFR

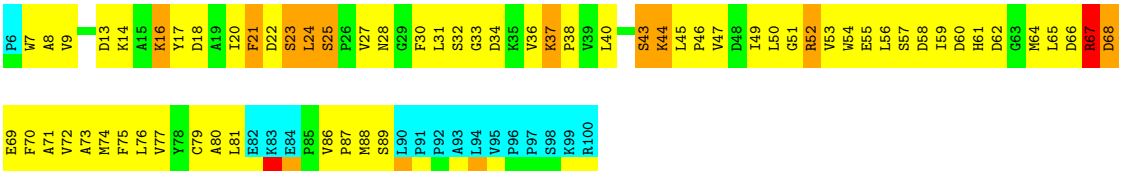
Chain B:

4.2.13 Score per residue for model 13

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:





• Molecule 2: PTGSSSTNPFR

Chain B:

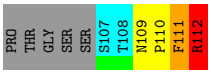
4.2.14 Score per residue for model 14

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:

• Molecule 2: PTGSSSTNPFR

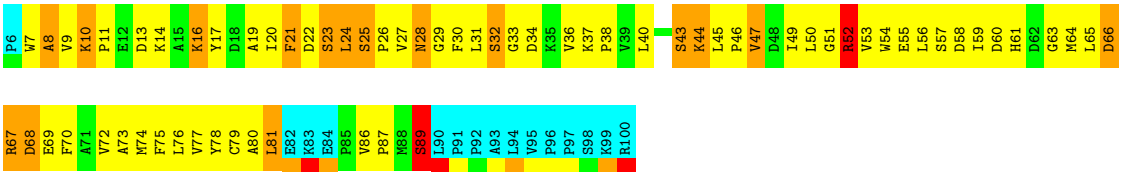
Chain B:



4.2.15 Score per residue for model 15

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:



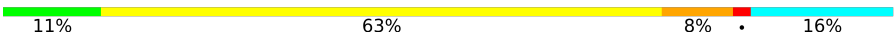
• Molecule 2: PTGSSSTNPFR

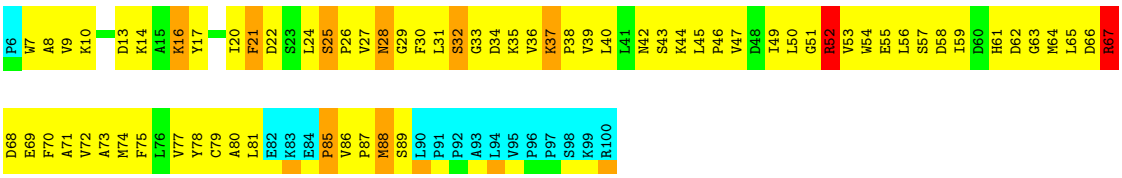
Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:





• Molecule 2: PTGSSSTNPFR

Chain B:

4.2.17 Score per residue for model 17

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:

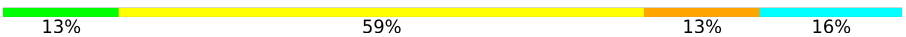
• Molecule 2: PTGSSSTNPFR

Chain B:

4.2.18 Score per residue for model 18

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:



• Molecule 2: PTGSSSTNPFR

Chain B:

4.2.19 Score per residue for model 19

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:

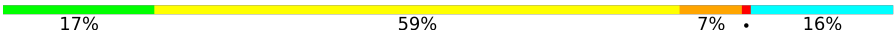
• Molecule 2: PTGSSSTNPFR

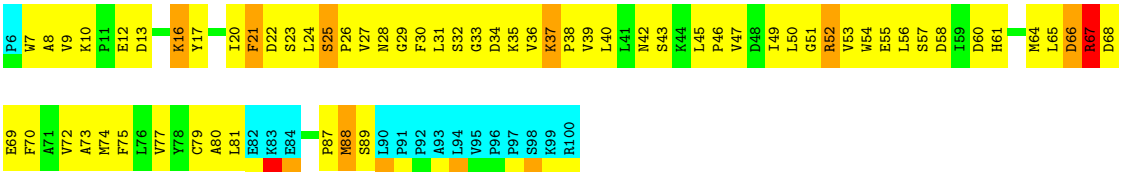
Chain B:

4.2.20 Score per residue for model 20

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR SUBSTRATE 15

Chain A:





• Molecule 2: PTGSSSTNPFR

Chain B:

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *20 LOWEST NOE ENERGIES*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.85
X-PLOR	refinement	3.85

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

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	1.9±0.4
2	B	0.0±0.0	0.9±0.2
All	All	0	56

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	67	ARG	Sidechain	19
2	B	112	ARG	Sidechain	19
1	A	52	ARG	Sidechain	18

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	626	624	625	135±9
2	B	38	35	35	18±3
All	All	13300	13199	13200	2768

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 104.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD12	1:A:31:LEU:HD13	1.12	1.14	4	20
1:A:53:VAL:HG11	1:A:77:VAL:HG23	1.11	1.23	3	20
1:A:36:VAL:HG21	1:A:65:LEU:HD12	1.04	1.24	13	9
1:A:45:LEU:HD11	1:A:80:ALA:HB3	1.01	1.26	7	19
1:A:24:LEU:HD12	1:A:31:LEU:CD1	1.01	1.85	19	20
1:A:53:VAL:HG11	1:A:77:VAL:CG2	0.97	1.87	16	20
1:A:57:SER:OG	1:A:65:LEU:HD21	0.95	1.60	11	2
1:A:40:LEU:HD12	2:B:111:PHE:CE2	0.93	1.98	15	20
1:A:36:VAL:HG11	1:A:65:LEU:HD12	0.93	1.39	15	18
1:A:57:SER:OG	1:A:73:ALA:HB2	0.92	1.65	2	15
1:A:52:ARG:O	1:A:56:LEU:HD12	0.91	1.66	17	20
1:A:43:SER:O	1:A:81:LEU:HD21	0.91	1.65	2	9
1:A:77:VAL:O	1:A:81:LEU:HD12	0.91	1.66	1	8
1:A:45:LEU:HD13	1:A:49:ILE:HG21	0.90	1.42	10	14
1:A:24:LEU:CD1	1:A:31:LEU:HD13	0.89	1.96	15	20
1:A:31:LEU:HD12	1:A:70:PHE:CD2	0.88	2.04	16	17
1:A:36:VAL:CG2	1:A:65:LEU:HD12	0.88	1.99	13	7
1:A:31:LEU:HD12	1:A:70:PHE:CD1	0.87	2.05	13	2
1:A:57:SER:CB	1:A:73:ALA:HB2	0.86	2.00	12	19
1:A:56:LEU:HD21	1:A:88:MET:C	0.86	1.91	12	16
1:A:40:LEU:HB3	1:A:50:LEU:HD22	0.85	1.46	14	20
1:A:36:VAL:HG12	1:A:40:LEU:CD1	0.84	2.02	16	20
1:A:53:VAL:CG1	1:A:77:VAL:HG23	0.83	2.03	16	4
1:A:45:LEU:HD11	1:A:80:ALA:CB	0.81	2.05	7	16
1:A:40:LEU:CD2	1:A:77:VAL:HG21	0.80	2.07	15	20
1:A:36:VAL:HG12	1:A:40:LEU:HD11	0.80	1.52	16	20
1:A:47:VAL:HG13	2:B:111:PHE:HB3	0.80	1.53	11	3
1:A:36:VAL:CG1	1:A:40:LEU:HD11	0.79	2.07	6	19
1:A:39:VAL:HG11	1:A:70:PHE:CZ	0.78	2.13	12	16
1:A:56:LEU:HD11	1:A:87:PRO:O	0.78	1.79	12	19
1:A:40:LEU:HD12	2:B:111:PHE:CZ	0.78	2.13	18	20
1:A:45:LEU:CD1	1:A:80:ALA:HB3	0.78	2.09	12	13
1:A:36:VAL:HG22	1:A:70:PHE:CE2	0.77	2.14	2	13
1:A:57:SER:HB3	1:A:73:ALA:HB2	0.77	1.57	19	1
1:A:40:LEU:HD22	1:A:77:VAL:HG21	0.76	1.57	15	10
1:A:72:VAL:O	1:A:76:LEU:HD12	0.76	1.80	3	9
1:A:81:LEU:HD23	1:A:81:LEU:N	0.76	1.96	14	7
1:A:36:VAL:HG11	1:A:65:LEU:CD1	0.75	2.12	13	18
1:A:45:LEU:CD1	1:A:81:LEU:HD21	0.74	2.11	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:CG1	1:A:65:LEU:HD12	0.74	2.12	8	18
1:A:20:ILE:HG22	1:A:70:PHE:CZ	0.74	2.18	3	18
1:A:57:SER:HB2	1:A:73:ALA:HB2	0.74	1.58	18	12
1:A:21:PHE:HA	1:A:31:LEU:HD11	0.73	1.60	14	20
1:A:45:LEU:HD22	1:A:49:ILE:HG13	0.72	1.61	3	20
1:A:81:LEU:HD12	1:A:81:LEU:N	0.71	2.01	7	4
1:A:73:ALA:O	1:A:77:VAL:HG23	0.71	1.86	4	11
1:A:24:LEU:HD21	1:A:39:VAL:CG2	0.70	2.15	3	3
1:A:53:VAL:HG13	1:A:76:LEU:HB3	0.70	1.62	13	8
1:A:47:VAL:HG11	2:B:111:PHE:O	0.69	1.88	11	11
1:A:68:ASP:O	1:A:71:ALA:HB3	0.68	1.89	16	8
1:A:36:VAL:HG22	1:A:70:PHE:CE1	0.68	2.24	13	2
1:A:47:VAL:HG13	2:B:111:PHE:CB	0.68	2.19	11	3
1:A:24:LEU:O	1:A:25:SER:CB	0.67	2.42	17	20
1:A:40:LEU:HD23	1:A:77:VAL:HG21	0.66	1.66	9	5
1:A:40:LEU:CD1	2:B:111:PHE:CE2	0.66	2.79	7	20
1:A:37:LYS:HG2	1:A:41:LEU:HD11	0.66	1.67	12	1
1:A:40:LEU:CD1	2:B:111:PHE:CZ	0.65	2.79	9	20
1:A:9:VAL:CG2	1:A:75:PHE:CD2	0.65	2.80	15	7
1:A:49:ILE:O	1:A:53:VAL:HG23	0.65	1.91	12	14
1:A:11:PRO:O	1:A:15:ALA:HB2	0.65	1.92	7	3
1:A:76:LEU:O	1:A:80:ALA:HB2	0.65	1.91	10	2
1:A:53:VAL:CG2	1:A:86:VAL:HG21	0.64	2.22	6	5
1:A:27:VAL:HG12	1:A:28:ASN:HD22	0.64	1.53	13	1
1:A:76:LEU:HD22	1:A:86:VAL:HG13	0.63	1.69	18	5
1:A:21:PHE:O	1:A:31:LEU:HD11	0.63	1.93	19	16
1:A:36:VAL:HG22	1:A:70:PHE:HE2	0.62	1.52	17	3
1:A:78:TYR:HA	1:A:81:LEU:HD13	0.62	1.69	18	1
1:A:50:LEU:HB3	2:B:111:PHE:CD2	0.62	2.30	14	18
1:A:86:VAL:HG13	1:A:87:PRO:HD2	0.62	1.71	15	1
1:A:60:ASP:O	1:A:61:HIS:CG	0.61	2.53	13	3
1:A:31:LEU:HD12	1:A:70:PHE:CE2	0.61	2.29	5	10
2:B:110:PRO:HG2	2:B:111:PHE:CE1	0.61	2.30	18	18
1:A:17:TYR:CD1	1:A:74:MET:CB	0.61	2.84	18	8
2:B:111:PHE:CD1	2:B:111:PHE:N	0.61	2.69	18	20
1:A:29:GLY:O	1:A:30:PHE:CD1	0.60	2.54	7	2
2:B:111:PHE:O	2:B:112:ARG:CG	0.60	2.49	18	2
1:A:45:LEU:HD13	1:A:49:ILE:CG2	0.60	2.22	10	9
1:A:13:ASP:O	1:A:17:TYR:CG	0.60	2.55	17	20
1:A:56:LEU:HD11	1:A:88:MET:HA	0.60	1.72	14	8
1:A:43:SER:HB2	1:A:81:LEU:HD11	0.59	1.73	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:VAL:CG2	1:A:86:VAL:HG11	0.59	2.26	13	5
1:A:9:VAL:HG22	1:A:75:PHE:CD2	0.59	2.33	15	5
1:A:16:LYS:HG2	1:A:17:TYR:CD1	0.59	2.33	2	17
1:A:13:ASP:O	1:A:17:TYR:CD1	0.59	2.56	13	15
1:A:43:SER:CB	1:A:77:VAL:CG1	0.59	2.80	2	14
1:A:54:TRP:CB	2:B:111:PHE:CE1	0.59	2.85	4	18
1:A:72:VAL:O	1:A:75:PHE:CE1	0.59	2.56	20	4
1:A:30:PHE:CE1	1:A:66:ASP:CB	0.58	2.86	12	1
1:A:54:TRP:CD1	1:A:54:TRP:C	0.58	2.76	14	20
1:A:58:ASP:O	1:A:61:HIS:CD2	0.58	2.57	4	6
1:A:54:TRP:CZ2	1:A:58:ASP:OD1	0.58	2.57	1	3
1:A:30:PHE:CE1	1:A:66:ASP:OD2	0.58	2.57	8	4
1:A:47:VAL:HG12	2:B:112:ARG:OXT	0.58	1.98	18	1
1:A:57:SER:OG	1:A:65:LEU:HD22	0.58	1.98	1	8
1:A:70:PHE:CE1	1:A:74:MET:SD	0.58	2.97	15	9
1:A:72:VAL:O	1:A:75:PHE:CE2	0.58	2.57	6	1
1:A:50:LEU:CB	2:B:111:PHE:CD2	0.58	2.87	9	17
1:A:30:PHE:CD1	1:A:66:ASP:OD1	0.57	2.57	4	2
1:A:20:ILE:HG22	1:A:70:PHE:CE1	0.57	2.34	20	12
1:A:49:ILE:HG21	1:A:80:ALA:HB1	0.57	1.76	15	1
1:A:45:LEU:CD1	1:A:80:ALA:CB	0.57	2.82	11	12
1:A:21:PHE:CA	1:A:31:LEU:HD11	0.57	2.29	6	17
1:A:81:LEU:N	1:A:81:LEU:CD2	0.57	2.64	9	4
1:A:39:VAL:HG11	1:A:70:PHE:HZ	0.57	1.58	7	6
1:A:30:PHE:CZ	1:A:66:ASP:OD2	0.57	2.57	8	3
1:A:75:PHE:C	1:A:75:PHE:CD1	0.57	2.78	15	3
1:A:16:LYS:CG	1:A:17:TYR:CD1	0.57	2.88	11	16
1:A:54:TRP:O	1:A:58:ASP:N	0.57	2.37	5	19
1:A:40:LEU:HD22	1:A:77:VAL:CG2	0.57	2.29	15	3
1:A:58:ASP:O	1:A:61:HIS:CE1	0.57	2.58	14	1
1:A:54:TRP:CE2	1:A:58:ASP:OD2	0.57	2.58	12	4
1:A:77:VAL:O	1:A:81:LEU:CD1	0.56	2.53	7	6
1:A:33:GLY:HA2	1:A:54:TRP:CZ3	0.56	2.34	9	13
1:A:60:ASP:C	1:A:61:HIS:CG	0.56	2.79	3	5
1:A:17:TYR:CE1	1:A:74:MET:HB3	0.56	2.35	19	11
1:A:54:TRP:HB2	2:B:111:PHE:CE1	0.56	2.35	9	15
1:A:21:PHE:CE2	1:A:67:ARG:N	0.56	2.73	16	16
1:A:37:LYS:CG	1:A:41:LEU:HD11	0.56	2.31	1	2
1:A:17:TYR:CD2	1:A:74:MET:HB2	0.56	2.36	9	10
1:A:36:VAL:HG21	1:A:65:LEU:CD1	0.56	2.14	13	1
1:A:47:VAL:CG1	2:B:111:PHE:O	0.56	2.53	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD11	1:A:81:LEU:CD2	0.56	2.30	6	2
1:A:21:PHE:HA	1:A:31:LEU:CD1	0.56	2.31	10	18
1:A:40:LEU:HD12	2:B:111:PHE:HE2	0.56	1.55	13	19
1:A:31:LEU:HD12	1:A:70:PHE:CE1	0.56	2.35	13	1
1:A:20:ILE:HG22	1:A:70:PHE:CE2	0.56	2.36	13	2
1:A:44:LYS:CG	1:A:44:LYS:O	0.56	2.54	3	2
2:B:109:ASN:OD1	2:B:112:ARG:N	0.56	2.36	18	3
1:A:60:ASP:O	1:A:61:HIS:CD2	0.56	2.58	13	1
1:A:28:ASN:ND2	1:A:30:PHE:CE2	0.56	2.74	19	1
1:A:17:TYR:CD1	1:A:17:TYR:N	0.56	2.70	12	20
1:A:56:LEU:CD1	1:A:87:PRO:O	0.56	2.54	7	15
1:A:78:TYR:HA	1:A:81:LEU:HD23	0.56	1.77	15	2
1:A:21:PHE:C	1:A:21:PHE:CD1	0.55	2.80	3	11
1:A:37:LYS:N	1:A:38:PRO:HD2	0.55	2.15	1	20
1:A:30:PHE:CD1	1:A:66:ASP:CB	0.55	2.90	12	1
1:A:43:SER:O	1:A:81:LEU:CD2	0.55	2.53	11	3
1:A:57:SER:O	1:A:69:GLU:CG	0.55	2.55	13	2
1:A:17:TYR:CD1	1:A:74:MET:HB3	0.55	2.37	3	8
1:A:17:TYR:CE1	1:A:74:MET:CB	0.55	2.90	18	4
1:A:40:LEU:C	1:A:50:LEU:HD13	0.55	2.22	1	15
1:A:27:VAL:HG12	1:A:28:ASN:ND2	0.55	2.17	13	1
1:A:17:TYR:CE1	1:A:74:MET:HB2	0.55	2.36	17	5
1:A:43:SER:OG	1:A:77:VAL:CG1	0.55	2.55	15	4
1:A:37:LYS:HA	2:B:111:PHE:CE2	0.54	2.37	18	19
1:A:36:VAL:HG21	1:A:65:LEU:HB2	0.54	1.79	18	5
1:A:57:SER:OG	1:A:65:LEU:CD2	0.54	2.56	1	7
1:A:24:LEU:HD21	1:A:39:VAL:HG23	0.54	1.79	16	2
1:A:57:SER:OG	1:A:73:ALA:CA	0.54	2.55	17	3
1:A:31:LEU:O	1:A:64:MET:HA	0.54	2.02	1	20
1:A:52:ARG:CD	1:A:87:PRO:O	0.54	2.55	9	4
1:A:45:LEU:HD11	1:A:81:LEU:HD21	0.54	1.78	6	1
1:A:45:LEU:CD1	1:A:81:LEU:CD2	0.54	2.85	5	2
1:A:66:ASP:N	1:A:66:ASP:OD1	0.54	2.38	6	3
2:B:111:PHE:O	2:B:112:ARG:CB	0.54	2.55	18	3
1:A:32:SER:O	1:A:35:LYS:N	0.54	2.39	6	12
1:A:80:ALA:C	1:A:81:LEU:HD23	0.54	2.23	9	4
1:A:28:ASN:O	1:A:28:ASN:ND2	0.54	2.40	15	15
1:A:30:PHE:CE1	1:A:66:ASP:HB3	0.54	2.38	12	5
1:A:59:ILE:N	1:A:69:GLU:OE2	0.54	2.41	12	8
1:A:33:GLY:O	1:A:37:LYS:N	0.54	2.40	15	3
1:A:66:ASP:OD1	1:A:66:ASP:N	0.54	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PHE:CZ	1:A:26:PRO:HB3	0.53	2.38	4	16
1:A:33:GLY:O	1:A:37:LYS:CB	0.53	2.57	1	12
1:A:49:ILE:O	1:A:53:VAL:CG2	0.53	2.56	2	8
1:A:52:ARG:CD	1:A:86:VAL:O	0.53	2.56	16	3
1:A:17:TYR:CD2	1:A:74:MET:CB	0.53	2.91	20	2
1:A:52:ARG:CG	1:A:88:MET:CG	0.53	2.86	18	1
1:A:55:GLU:CG	2:B:109:ASN:ND2	0.53	2.71	9	1
1:A:66:ASP:OD1	1:A:67:ARG:N	0.53	2.41	10	3
1:A:75:PHE:CE1	1:A:76:LEU:HG	0.53	2.39	15	2
1:A:53:VAL:HG22	1:A:86:VAL:HG11	0.53	1.80	13	1
1:A:56:LEU:HD21	1:A:89:SER:N	0.53	2.18	6	12
1:A:17:TYR:CZ	1:A:74:MET:HB2	0.53	2.38	17	5
1:A:70:PHE:O	1:A:74:MET:CG	0.53	2.56	13	5
2:B:109:ASN:N	2:B:109:ASN:OD1	0.53	2.39	9	1
1:A:51:GLY:CA	2:B:109:ASN:OD1	0.53	2.57	16	2
1:A:29:GLY:O	1:A:66:ASP:CB	0.53	2.57	5	3
1:A:70:PHE:CD1	1:A:74:MET:SD	0.53	3.02	16	3
1:A:21:PHE:CD1	1:A:21:PHE:C	0.53	2.82	13	7
1:A:30:PHE:CD1	1:A:66:ASP:HB3	0.53	2.39	3	5
1:A:70:PHE:O	1:A:74:MET:SD	0.52	2.68	15	9
1:A:73:ALA:O	1:A:77:VAL:CG2	0.52	2.57	12	6
1:A:66:ASP:O	1:A:69:GLU:N	0.52	2.42	12	3
1:A:12:GLU:O	1:A:16:LYS:CG	0.52	2.57	20	1
1:A:31:LEU:O	1:A:64:MET:CA	0.52	2.57	12	9
1:A:43:SER:HB3	1:A:77:VAL:CG1	0.52	2.33	16	9
1:A:47:VAL:CG1	2:B:111:PHE:C	0.52	2.78	11	11
1:A:54:TRP:NE1	1:A:58:ASP:OD2	0.52	2.42	12	2
1:A:40:LEU:CD2	1:A:77:VAL:CG2	0.52	2.87	9	2
1:A:61:HIS:ND1	1:A:61:HIS:O	0.52	2.42	13	2
1:A:66:ASP:OD1	1:A:68:ASP:N	0.52	2.41	14	4
1:A:81:LEU:N	1:A:81:LEU:CD1	0.52	2.71	7	1
1:A:37:LYS:HG3	1:A:41:LEU:HD11	0.52	1.81	14	3
1:A:47:VAL:HG13	2:B:111:PHE:C	0.52	2.25	16	12
1:A:54:TRP:CD1	1:A:55:GLU:N	0.52	2.78	16	18
1:A:60:ASP:N	1:A:69:GLU:OE2	0.52	2.42	19	2
1:A:27:VAL:O	1:A:28:ASN:CB	0.52	2.58	16	12
1:A:54:TRP:O	1:A:57:SER:N	0.52	2.43	9	6
1:A:66:ASP:OD1	1:A:69:GLU:CG	0.52	2.57	20	1
1:A:36:VAL:HG22	1:A:70:PHE:HE1	0.52	1.61	13	2
1:A:49:ILE:O	1:A:53:VAL:N	0.52	2.41	6	13
1:A:31:LEU:CD1	1:A:70:PHE:CE1	0.52	2.92	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:MET:SD	1:A:74:MET:N	0.52	2.83	17	9
1:A:21:PHE:CE1	1:A:26:PRO:HB3	0.52	2.40	19	2
1:A:57:SER:OG	1:A:73:ALA:CB	0.52	2.57	8	5
1:A:17:TYR:CD1	1:A:74:MET:HB2	0.52	2.39	16	4
1:A:62:ASP:N	1:A:62:ASP:OD1	0.52	2.43	9	3
1:A:53:VAL:HG23	1:A:86:VAL:HG11	0.52	1.80	9	3
1:A:17:TYR:CG	1:A:74:MET:HB2	0.52	2.40	16	2
1:A:36:VAL:HG22	1:A:70:PHE:CD2	0.51	2.41	2	3
1:A:78:TYR:HA	1:A:81:LEU:CD1	0.51	2.35	11	2
1:A:72:VAL:HA	1:A:75:PHE:CE2	0.51	2.40	15	4
1:A:52:ARG:NH1	1:A:86:VAL:O	0.51	2.43	18	1
1:A:13:ASP:O	1:A:17:TYR:CD2	0.51	2.63	15	5
1:A:54:TRP:CE2	1:A:58:ASP:OD1	0.51	2.63	1	1
1:A:52:ARG:CG	1:A:88:MET:HG2	0.51	2.35	18	5
1:A:25:SER:O	1:A:25:SER:OG	0.51	2.29	8	4
1:A:60:ASP:O	1:A:61:HIS:ND1	0.51	2.44	2	2
1:A:77:VAL:O	1:A:81:LEU:HG	0.51	2.05	3	9
1:A:60:ASP:O	1:A:61:HIS:CB	0.51	2.58	14	2
1:A:65:LEU:HD13	1:A:70:PHE:HA	0.51	1.82	18	2
1:A:17:TYR:CD2	1:A:71:ALA:HA	0.51	2.40	1	6
1:A:60:ASP:OD1	1:A:62:ASP:N	0.51	2.43	1	3
1:A:7:TRP:O	1:A:9:VAL:N	0.51	2.43	15	11
1:A:54:TRP:CZ3	1:A:65:LEU:HG	0.51	2.41	9	9
1:A:57:SER:O	1:A:59:ILE:N	0.51	2.44	11	2
1:A:31:LEU:O	1:A:65:LEU:N	0.51	2.41	11	6
1:A:28:ASN:O	1:A:30:PHE:CD2	0.51	2.64	19	1
1:A:10:LYS:CB	1:A:11:PRO:HD2	0.50	2.37	4	9
1:A:17:TYR:CE2	1:A:74:MET:HB2	0.50	2.41	7	7
1:A:62:ASP:OD1	1:A:62:ASP:N	0.50	2.44	17	7
1:A:52:ARG:O	1:A:56:LEU:CD1	0.50	2.56	13	3
1:A:43:SER:CB	1:A:77:VAL:HG13	0.50	2.37	15	8
1:A:56:LEU:CD2	1:A:89:SER:C	0.50	2.80	11	4
1:A:76:LEU:O	1:A:80:ALA:CB	0.50	2.59	10	2
1:A:67:ARG:CG	1:A:68:ASP:N	0.50	2.74	17	5
1:A:61:HIS:CD2	1:A:61:HIS:N	0.50	2.79	4	5
1:A:31:LEU:CD1	1:A:70:PHE:CE2	0.50	2.94	5	7
2:B:112:ARG:CG	2:B:112:ARG:OXT	0.50	2.60	14	1
1:A:77:VAL:O	1:A:81:LEU:CG	0.50	2.60	5	2
1:A:74:MET:HA	1:A:74:MET:CE	0.50	2.37	4	8
1:A:25:SER:O	1:A:35:LYS:NZ	0.50	2.43	10	2
1:A:66:ASP:OD2	1:A:69:GLU:CG	0.50	2.59	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ASP:OD1	1:A:34:ASP:N	0.50	2.45	6	1
1:A:75:PHE:CZ	1:A:76:LEU:HG	0.50	2.42	9	7
1:A:52:ARG:CD	1:A:88:MET:HG2	0.50	2.36	3	6
1:A:43:SER:O	1:A:44:LYS:CB	0.50	2.60	4	6
1:A:60:ASP:C	1:A:61:HIS:CD2	0.50	2.84	6	3
1:A:60:ASP:OD1	1:A:61:HIS:N	0.50	2.44	11	2
2:B:110:PRO:HD2	2:B:111:PHE:CE1	0.49	2.42	9	13
1:A:30:PHE:CE1	1:A:66:ASP:HB2	0.49	2.41	15	3
1:A:7:TRP:CE2	1:A:9:VAL:HB	0.49	2.41	2	17
1:A:51:GLY:O	2:B:109:ASN:ND2	0.49	2.45	6	5
1:A:54:TRP:CZ2	1:A:58:ASP:OD2	0.49	2.64	12	6
1:A:7:TRP:CZ2	1:A:68:ASP:OD1	0.49	2.65	19	1
1:A:43:SER:OG	1:A:77:VAL:HG11	0.49	2.07	19	1
1:A:63:GLY:C	1:A:64:MET:CG	0.49	2.80	15	5
1:A:60:ASP:N	1:A:60:ASP:OD1	0.49	2.43	2	1
1:A:58:ASP:OD1	1:A:61:HIS:N	0.49	2.45	10	1
1:A:40:LEU:CB	1:A:50:LEU:HD13	0.49	2.37	20	5
1:A:27:VAL:O	1:A:28:ASN:OD1	0.49	2.31	16	3
1:A:16:LYS:O	1:A:20:ILE:HD12	0.49	2.07	2	2
1:A:53:VAL:O	1:A:57:SER:CB	0.49	2.60	4	6
1:A:78:TYR:HA	1:A:81:LEU:CD2	0.49	2.38	15	2
1:A:66:ASP:CG	1:A:67:ARG:N	0.49	2.66	1	3
1:A:45:LEU:HG	1:A:81:LEU:CD2	0.49	2.38	6	5
1:A:11:PRO:O	1:A:15:ALA:CB	0.49	2.60	7	1
1:A:86:VAL:CG1	1:A:87:PRO:HD2	0.49	2.38	15	1
1:A:17:TYR:CG	1:A:74:MET:CB	0.49	2.96	20	5
1:A:32:SER:CA	1:A:64:MET:SD	0.49	3.01	10	2
1:A:45:LEU:HD11	1:A:81:LEU:N	0.49	2.22	10	2
1:A:70:PHE:O	1:A:74:MET:HG2	0.49	2.07	2	18
1:A:62:ASP:OD1	1:A:64:MET:N	0.49	2.46	12	1
1:A:10:LYS:CG	1:A:11:PRO:HD2	0.48	2.38	1	5
1:A:27:VAL:O	1:A:28:ASN:HB3	0.48	2.08	11	16
1:A:13:ASP:O	1:A:17:TYR:CE1	0.48	2.66	13	1
1:A:52:ARG:NE	1:A:88:MET:HG2	0.48	2.24	2	1
1:A:68:ASP:CG	1:A:69:GLU:N	0.48	2.67	18	2
1:A:21:PHE:HB2	1:A:70:PHE:CD2	0.48	2.43	13	2
1:A:21:PHE:CD2	1:A:67:ARG:HA	0.48	2.44	6	12
1:A:29:GLY:O	1:A:66:ASP:OD1	0.48	2.32	10	4
1:A:24:LEU:CD1	1:A:31:LEU:CD1	0.48	2.79	13	3
1:A:24:LEU:HD11	1:A:39:VAL:HG21	0.48	1.85	7	2
1:A:75:PHE:CD1	1:A:75:PHE:C	0.48	2.87	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ARG:NH2	1:A:88:MET:SD	0.48	2.87	13	1
1:A:16:LYS:HG2	1:A:17:TYR:CE1	0.48	2.44	3	5
1:A:24:LEU:HD12	1:A:31:LEU:HD11	0.48	1.81	9	2
1:A:24:LEU:O	1:A:25:SER:OG	0.48	2.31	8	7
1:A:51:GLY:HA2	2:B:109:ASN:OD1	0.48	2.09	18	10
1:A:53:VAL:HG13	1:A:76:LEU:CB	0.48	2.38	6	3
1:A:14:LYS:NZ	1:A:68:ASP:OD2	0.48	2.47	3	1
1:A:33:GLY:O	1:A:37:LYS:HB3	0.48	2.08	5	4
1:A:32:SER:O	1:A:34:ASP:N	0.48	2.47	16	18
1:A:14:LYS:HG2	1:A:71:ALA:HB1	0.48	1.85	13	1
1:A:17:TYR:CZ	1:A:74:MET:HB3	0.48	2.44	20	1
1:A:60:ASP:OD2	1:A:69:GLU:OE2	0.47	2.32	17	4
1:A:32:SER:CB	1:A:64:MET:SD	0.47	3.02	10	2
1:A:52:ARG:C	1:A:56:LEU:HD12	0.47	2.27	12	1
1:A:7:TRP:CH2	1:A:14:LYS:HG3	0.47	2.43	13	1
1:A:52:ARG:CG	1:A:88:MET:HG3	0.47	2.39	16	1
1:A:47:VAL:O	2:B:112:ARG:O	0.47	2.32	20	1
1:A:25:SER:OG	1:A:25:SER:O	0.47	2.31	9	1
1:A:14:LYS:O	1:A:18:ASP:CB	0.47	2.62	12	1
1:A:46:PRO:HD2	1:A:49:ILE:CG1	0.47	2.39	14	20
1:A:52:ARG:HD3	1:A:87:PRO:O	0.47	2.10	5	2
1:A:60:ASP:OD2	1:A:69:GLU:OE1	0.47	2.33	2	6
1:A:9:VAL:CG2	1:A:75:PHE:CE2	0.47	2.98	15	1
1:A:29:GLY:O	1:A:66:ASP:HB2	0.47	2.09	16	3
1:A:59:ILE:N	1:A:69:GLU:OE1	0.47	2.48	11	2
1:A:29:GLY:C	1:A:30:PHE:CD2	0.47	2.88	19	5
1:A:32:SER:O	1:A:33:GLY:C	0.47	2.53	15	20
1:A:47:VAL:O	1:A:51:GLY:N	0.47	2.46	1	5
1:A:49:ILE:O	1:A:53:VAL:CB	0.47	2.62	1	4
1:A:47:VAL:HG13	2:B:111:PHE:CA	0.47	2.39	14	5
1:A:51:GLY:N	2:B:111:PHE:HB2	0.47	2.25	14	1
1:A:36:VAL:O	1:A:39:VAL:N	0.47	2.48	1	5
1:A:53:VAL:HG23	1:A:86:VAL:HG21	0.47	1.84	5	1
1:A:33:GLY:O	1:A:37:LYS:HB2	0.47	2.10	14	4
1:A:52:ARG:HG2	1:A:87:PRO:O	0.47	2.10	14	1
1:A:30:PHE:HB3	1:A:64:MET:CE	0.47	2.40	10	2
1:A:78:TYR:HA	1:A:81:LEU:HD12	0.47	1.87	11	1
1:A:20:ILE:CD1	1:A:74:MET:SD	0.47	3.03	3	1
1:A:75:PHE:O	1:A:79:CYS:CB	0.47	2.63	15	1
1:A:52:ARG:HG3	1:A:88:MET:CG	0.47	2.40	18	1
1:A:30:PHE:CD1	1:A:66:ASP:HB2	0.46	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:O	1:A:44:LYS:HG2	0.46	2.09	3	2
1:A:51:GLY:CA	2:B:111:PHE:HB2	0.46	2.40	7	6
1:A:28:ASN:O	1:A:30:PHE:CE2	0.46	2.68	19	1
1:A:37:LYS:CG	1:A:41:LEU:CD1	0.46	2.94	1	2
1:A:22:ASP:O	1:A:22:ASP:OD1	0.46	2.33	12	4
1:A:37:LYS:HG3	1:A:41:LEU:CD1	0.46	2.40	19	3
1:A:60:ASP:OD1	1:A:62:ASP:OD1	0.46	2.34	3	3
1:A:43:SER:HB3	1:A:81:LEU:HD11	0.46	1.86	12	1
1:A:52:ARG:HD2	1:A:86:VAL:O	0.46	2.10	18	10
1:A:53:VAL:HG22	1:A:76:LEU:HB3	0.46	1.87	3	1
1:A:30:PHE:CE1	1:A:66:ASP:CG	0.46	2.89	4	1
1:A:30:PHE:CD1	1:A:66:ASP:CG	0.46	2.89	7	1
1:A:21:PHE:CD1	1:A:22:ASP:N	0.46	2.84	13	12
1:A:60:ASP:O	1:A:61:HIS:HB2	0.46	2.10	12	9
1:A:29:GLY:O	1:A:66:ASP:CG	0.46	2.54	8	3
1:A:52:ARG:HD3	1:A:88:MET:CG	0.46	2.41	2	4
1:A:7:TRP:O	1:A:8:ALA:C	0.46	2.54	9	12
1:A:53:VAL:O	1:A:57:SER:HB3	0.46	2.11	14	6
1:A:31:LEU:O	1:A:64:MET:CB	0.46	2.64	9	1
1:A:63:GLY:C	1:A:64:MET:HG2	0.46	2.31	12	3
1:A:19:ALA:O	1:A:23:SER:CB	0.46	2.64	2	3
1:A:24:LEU:O	1:A:25:SER:HB3	0.46	2.10	6	5
1:A:60:ASP:C	1:A:61:HIS:ND1	0.46	2.69	3	1
1:A:12:GLU:O	1:A:16:LYS:HG3	0.46	2.11	20	2
1:A:37:LYS:N	1:A:38:PRO:CD	0.46	2.78	1	13
1:A:21:PHE:CE1	1:A:26:PRO:HG3	0.46	2.45	7	1
1:A:28:ASN:O	1:A:28:ASN:CG	0.45	2.55	20	4
1:A:36:VAL:O	1:A:37:LYS:C	0.45	2.54	11	15
1:A:66:ASP:O	1:A:67:ARG:C	0.45	2.53	3	11
1:A:52:ARG:NE	1:A:86:VAL:O	0.45	2.50	6	1
1:A:37:LYS:HG2	1:A:41:LEU:CD1	0.45	2.41	12	1
1:A:66:ASP:OD2	1:A:69:GLU:OE1	0.45	2.33	3	2
1:A:17:TYR:O	1:A:21:PHE:HB3	0.45	2.11	8	3
2:B:109:ASN:ND2	2:B:111:PHE:CD1	0.45	2.84	8	2
1:A:60:ASP:OD2	1:A:62:ASP:OD2	0.45	2.34	7	1
1:A:20:ILE:O	1:A:24:LEU:HG	0.45	2.12	5	2
1:A:37:LYS:O	1:A:41:LEU:HG	0.45	2.12	14	6
1:A:21:PHE:HB2	1:A:70:PHE:CD1	0.45	2.45	4	2
1:A:45:LEU:CG	1:A:81:LEU:HD21	0.45	2.41	6	1
1:A:11:PRO:O	1:A:15:ALA:N	0.45	2.50	7	1
1:A:20:ILE:CG2	1:A:70:PHE:CE1	0.45	2.99	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:SER:O	1:A:69:GLU:HG2	0.45	2.11	17	5
1:A:54:TRP:CZ2	1:A:58:ASP:CG	0.45	2.89	17	1
1:A:20:ILE:O	1:A:23:SER:OG	0.45	2.33	9	2
1:A:37:LYS:HB3	1:A:38:PRO:CD	0.45	2.42	11	9
1:A:44:LYS:HA	1:A:44:LYS:CE	0.45	2.42	5	1
1:A:28:ASN:ND2	1:A:30:PHE:CD2	0.45	2.85	19	1
1:A:40:LEU:O	1:A:43:SER:OG	0.45	2.33	16	1
1:A:17:TYR:OH	1:A:75:PHE:CB	0.45	2.64	13	2
1:A:32:SER:C	1:A:34:ASP:N	0.45	2.70	8	20
1:A:67:ARG:HG3	1:A:68:ASP:N	0.45	2.27	14	6
1:A:16:LYS:CG	1:A:17:TYR:CE1	0.45	2.99	15	4
1:A:20:ILE:HG22	1:A:70:PHE:HZ	0.45	1.68	3	1
1:A:52:ARG:HD2	1:A:87:PRO:O	0.45	2.12	6	3
1:A:40:LEU:CB	1:A:50:LEU:HD22	0.44	2.35	3	1
1:A:55:GLU:HG2	2:B:109:ASN:ND2	0.44	2.27	5	1
1:A:66:ASP:OD1	1:A:66:ASP:C	0.44	2.56	16	3
1:A:24:LEU:N	1:A:24:LEU:HD23	0.44	2.27	13	1
1:A:49:ILE:O	1:A:53:VAL:HB	0.44	2.12	13	3
1:A:58:ASP:OD1	1:A:64:MET:O	0.44	2.36	17	2
1:A:52:ARG:CD	1:A:87:PRO:C	0.44	2.85	20	1
1:A:14:LYS:HA	1:A:17:TYR:CD2	0.44	2.47	6	2
1:A:54:TRP:CE3	1:A:65:LEU:HD11	0.44	2.47	13	1
1:A:60:ASP:OD2	1:A:69:GLU:CD	0.44	2.56	15	2
1:A:39:VAL:O	1:A:42:ASN:OD1	0.44	2.34	16	1
1:A:70:PHE:CE1	1:A:74:MET:CE	0.44	3.00	19	1
2:B:109:ASN:OD1	2:B:112:ARG:HA	0.44	2.12	20	2
1:A:21:PHE:HB2	1:A:70:PHE:CG	0.44	2.47	9	4
1:A:37:LYS:O	1:A:41:LEU:CG	0.44	2.65	14	2
1:A:47:VAL:CG2	2:B:111:PHE:O	0.44	2.65	15	1
1:A:60:ASP:O	1:A:61:HIS:C	0.44	2.55	2	2
1:A:63:GLY:C	1:A:64:MET:HG3	0.44	2.33	4	3
1:A:54:TRP:HB2	2:B:111:PHE:CZ	0.44	2.47	8	1
1:A:31:LEU:C	1:A:64:MET:SD	0.44	2.96	13	1
1:A:52:ARG:HG2	1:A:88:MET:CG	0.44	2.43	16	1
1:A:53:VAL:O	1:A:57:SER:OG	0.44	2.31	19	2
1:A:24:LEU:HD11	1:A:70:PHE:CZ	0.44	2.48	13	1
1:A:12:GLU:HG3	1:A:13:ASP:N	0.44	2.28	6	5
1:A:52:ARG:CD	1:A:88:MET:CG	0.44	2.96	3	1
1:A:12:GLU:CG	1:A:13:ASP:N	0.44	2.80	7	1
1:A:66:ASP:OD1	1:A:68:ASP:OD1	0.44	2.36	16	1
1:A:42:ASN:O	1:A:42:ASN:OD1	0.44	2.35	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:GLY:O	1:A:55:GLU:HG3	0.43	2.13	8	5
1:A:37:LYS:CD	2:B:110:PRO:HB2	0.43	2.43	9	4
1:A:21:PHE:CZ	1:A:67:ARG:HB3	0.43	2.49	18	2
1:A:30:PHE:CE1	1:A:66:ASP:OD1	0.43	2.71	4	1
1:A:60:ASP:OD2	1:A:62:ASP:CG	0.43	2.56	8	1
1:A:32:SER:HA	1:A:64:MET:SD	0.43	2.53	10	2
1:A:29:GLY:O	1:A:66:ASP:OD2	0.43	2.36	15	1
1:A:32:SER:OG	1:A:35:LYS:HE2	0.43	2.13	17	1
1:A:24:LEU:C	1:A:25:SER:OG	0.43	2.57	18	2
1:A:75:PHE:O	1:A:79:CYS:SG	0.43	2.76	2	3
1:A:20:ILE:HD13	1:A:74:MET:SD	0.43	2.52	3	1
1:A:54:TRP:O	1:A:55:GLU:C	0.43	2.56	9	2
1:A:52:ARG:CZ	1:A:88:MET:HG2	0.43	2.43	13	1
1:A:63:GLY:O	1:A:64:MET:HG2	0.43	2.14	14	2
1:A:66:ASP:OD2	1:A:69:GLU:CD	0.43	2.57	14	1
2:B:111:PHE:O	2:B:112:ARG:HG2	0.43	2.13	18	3
1:A:24:LEU:O	1:A:25:SER:HB2	0.43	2.11	2	5
1:A:42:ASN:OD1	1:A:42:ASN:C	0.43	2.57	16	1
1:A:60:ASP:OD1	1:A:62:ASP:CG	0.43	2.57	3	2
1:A:43:SER:O	1:A:44:LYS:HB3	0.43	2.14	5	3
1:A:77:VAL:O	1:A:81:LEU:CD2	0.43	2.67	3	2
1:A:37:LYS:HB3	1:A:38:PRO:HD3	0.43	1.91	6	9
1:A:43:SER:HB2	1:A:77:VAL:CG1	0.43	2.43	8	1
1:A:55:GLU:CG	2:B:109:ASN:HD21	0.43	2.26	9	1
1:A:60:ASP:CG	1:A:69:GLU:OE2	0.43	2.57	20	3
1:A:62:ASP:OD1	1:A:62:ASP:C	0.43	2.55	12	1
1:A:13:ASP:HB3	1:A:17:TYR:CZ	0.43	2.49	20	1
1:A:12:GLU:HG2	1:A:13:ASP:N	0.43	2.28	8	1
1:A:55:GLU:HG3	2:B:109:ASN:ND2	0.43	2.29	18	1
1:A:63:GLY:O	1:A:64:MET:HG3	0.43	2.14	2	6
1:A:68:ASP:O	1:A:68:ASP:OD1	0.42	2.37	2	1
1:A:20:ILE:CG2	1:A:70:PHE:CZ	0.42	3.00	3	1
1:A:40:LEU:C	1:A:50:LEU:CD1	0.42	2.87	16	2
1:A:60:ASP:OD1	1:A:60:ASP:C	0.42	2.55	7	1
1:A:66:ASP:HB2	1:A:69:GLU:OE1	0.42	2.14	10	1
1:A:17:TYR:OH	1:A:75:PHE:HB3	0.42	2.14	13	1
1:A:10:LYS:CB	1:A:11:PRO:CD	0.42	2.97	18	3
1:A:24:LEU:CD2	1:A:39:VAL:CG2	0.42	2.94	3	1
1:A:14:LYS:O	1:A:14:LYS:HD3	0.42	2.14	10	1
1:A:47:VAL:O	2:B:112:ARG:OXT	0.42	2.36	18	1
1:A:37:LYS:HD2	2:B:110:PRO:O	0.42	2.13	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LYS:CB	1:A:38:PRO:CD	0.42	2.96	20	6
1:A:45:LEU:CG	1:A:81:LEU:CD2	0.42	2.97	6	2
1:A:55:GLU:OE2	2:B:112:ARG:NH2	0.42	2.51	13	1
1:A:59:ILE:HG12	1:A:69:GLU:HG2	0.42	1.92	2	1
1:A:52:ARG:NH1	1:A:88:MET:HG2	0.42	2.29	9	1
1:A:31:LEU:O	1:A:64:MET:HB3	0.42	2.15	12	1
1:A:59:ILE:CG1	1:A:69:GLU:HG2	0.42	2.44	16	1
1:A:66:ASP:OD1	1:A:69:GLU:N	0.42	2.46	13	3
1:A:66:ASP:N	1:A:69:GLU:HB2	0.42	2.29	7	2
1:A:29:GLY:O	1:A:30:PHE:CG	0.42	2.72	12	3
1:A:9:VAL:HG13	1:A:13:ASP:HB3	0.42	1.91	18	1
1:A:54:TRP:CE2	1:A:58:ASP:HB2	0.42	2.50	10	1
1:A:58:ASP:O	1:A:61:HIS:ND1	0.42	2.52	14	1
1:A:35:LYS:O	1:A:38:PRO:HG2	0.42	2.15	16	2
1:A:9:VAL:HG12	1:A:10:LYS:N	0.42	2.29	20	1
1:A:77:VAL:O	1:A:81:LEU:HD21	0.42	2.14	3	1
1:A:24:LEU:HB3	1:A:35:LYS:HB3	0.42	1.91	14	1
1:A:24:LEU:O	1:A:35:LYS:HE3	0.42	2.15	18	1
1:A:68:ASP:OD1	1:A:68:ASP:C	0.42	2.58	2	1
1:A:47:VAL:CG1	1:A:47:VAL:O	0.42	2.68	5	5
1:A:64:MET:HE3	1:A:64:MET:HB3	0.42	1.85	10	1
1:A:74:MET:HA	1:A:74:MET:HE3	0.42	1.92	16	1
1:A:60:ASP:OD2	1:A:62:ASP:HB3	0.42	2.14	8	1
1:A:27:VAL:O	1:A:28:ASN:HB2	0.42	2.15	13	1
1:A:52:ARG:CD	1:A:88:MET:HG3	0.42	2.45	18	1
1:A:54:TRP:O	1:A:57:SER:HB3	0.41	2.15	3	3
1:A:52:ARG:HD3	1:A:87:PRO:C	0.41	2.35	6	1
1:A:54:TRP:CG	2:B:111:PHE:CE1	0.41	3.08	8	2
1:A:23:SER:C	1:A:24:LEU:HD23	0.41	2.35	13	1
1:A:66:ASP:OD1	1:A:68:ASP:CG	0.41	2.59	16	1
1:A:66:ASP:OD1	1:A:69:GLU:CB	0.41	2.68	20	1
1:A:67:ARG:HG3	1:A:68:ASP:OD1	0.41	2.15	3	1
1:A:57:SER:O	1:A:69:GLU:HG3	0.41	2.14	13	1
1:A:39:VAL:HG21	1:A:70:PHE:HZ	0.41	1.75	14	1
1:A:75:PHE:O	1:A:79:CYS:HB2	0.41	2.15	15	1
1:A:43:SER:O	1:A:44:LYS:HB2	0.41	2.15	19	2
1:A:42:ASN:OD1	1:A:43:SER:N	0.41	2.53	16	1
1:A:58:ASP:HA	1:A:69:GLU:OE2	0.41	2.16	2	1
1:A:24:LEU:CB	1:A:35:LYS:HB3	0.41	2.45	14	2
1:A:36:VAL:O	1:A:39:VAL:HB	0.41	2.14	1	3
1:A:36:VAL:HA	1:A:39:VAL:HB	0.41	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:VAL:O	1:A:47:VAL:CG1	0.41	2.68	3	3
1:A:17:TYR:CG	1:A:74:MET:CG	0.41	3.04	6	1
1:A:24:LEU:O	1:A:35:LYS:HD3	0.41	2.14	7	2
1:A:47:VAL:HG21	2:B:111:PHE:O	0.41	2.15	15	1
1:A:66:ASP:CG	1:A:68:ASP:OD1	0.41	2.58	16	1
1:A:66:ASP:OD2	1:A:69:GLU:HG3	0.41	2.14	14	2
1:A:46:PRO:O	1:A:50:LEU:HG	0.41	2.15	14	3
1:A:7:TRP:CZ3	1:A:14:LYS:HE2	0.41	2.51	12	1
2:B:109:ASN:OD1	2:B:112:ARG:CA	0.41	2.69	20	1
2:B:111:PHE:O	2:B:112:ARG:HB3	0.41	2.15	14	1
1:A:57:SER:OG	1:A:73:ALA:HA	0.41	2.16	19	1
1:A:7:TRP:CH2	1:A:68:ASP:OD1	0.41	2.73	6	1
1:A:51:GLY:O	1:A:55:GLU:OE1	0.41	2.39	8	1
1:A:57:SER:HB2	1:A:73:ALA:CB	0.41	2.44	13	1
1:A:51:GLY:HA2	2:B:111:PHE:HB2	0.41	1.93	8	2
1:A:45:LEU:HD11	1:A:81:LEU:HD23	0.41	1.93	5	1
1:A:21:PHE:CD2	1:A:31:LEU:HG	0.41	2.51	6	1
1:A:45:LEU:HG	1:A:81:LEU:HD21	0.41	1.93	6	1
1:A:10:LYS:O	1:A:14:LYS:N	0.41	2.47	7	1
1:A:10:LYS:HB3	1:A:11:PRO:HD2	0.41	1.92	8	1
1:A:17:TYR:CB	1:A:74:MET:HG3	0.41	2.46	9	1
1:A:54:TRP:O	1:A:57:SER:HB2	0.41	2.16	9	2
1:A:62:ASP:OD2	1:A:64:MET:HB2	0.41	2.16	9	1
1:A:7:TRP:HH2	1:A:14:LYS:HZ2	0.41	1.55	14	1
1:A:19:ALA:O	1:A:23:SER:HB3	0.41	2.16	15	1
1:A:36:VAL:HG11	1:A:65:LEU:HD11	0.41	1.91	13	2
1:A:7:TRP:C	1:A:9:VAL:N	0.41	2.74	9	2
1:A:7:TRP:CD2	1:A:9:VAL:HB	0.41	2.51	17	1
1:A:66:ASP:N	1:A:69:GLU:HB3	0.41	2.31	17	1
1:A:60:ASP:OD1	1:A:62:ASP:CB	0.40	2.69	1	1
1:A:65:LEU:HD23	1:A:65:LEU:HA	0.40	1.74	8	1
1:A:70:PHE:CE2	1:A:74:MET:SD	0.40	3.14	13	1
1:A:58:ASP:O	1:A:59:ILE:C	0.40	2.56	14	1
1:A:7:TRP:O	1:A:9:VAL:O	0.40	2.38	20	1
1:A:66:ASP:OD1	1:A:69:GLU:HG3	0.40	2.15	20	1
1:A:57:SER:OG	1:A:58:ASP:N	0.40	2.54	11	1
1:A:57:SER:O	1:A:69:GLU:HB3	0.40	2.16	15	1
1:A:86:VAL:CG1	1:A:87:PRO:CD	0.40	2.99	15	1
2:B:111:PHE:O	2:B:112:ARG:C	0.40	2.59	8	1
1:A:19:ALA:O	1:A:23:SER:HB2	0.40	2.15	12	1
1:A:33:GLY:O	1:A:37:LYS:HG3	0.40	2.17	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:CG1	1:A:69:GLU:HG3	0.40	2.47	6	1
1:A:21:PHE:CZ	1:A:26:PRO:CB	0.40	3.04	7	1
1:A:13:ASP:HB3	1:A:17:TYR:CE2	0.40	2.51	17	1
1:A:31:LEU:HD23	1:A:31:LEU:HA	0.40	1.75	17	1
1:A:31:LEU:O	1:A:64:MET:SD	0.40	2.79	13	1
1:A:36:VAL:CG1	1:A:65:LEU:CD1	0.40	2.93	13	1
1:A:36:VAL:CB	1:A:65:LEU:HD12	0.40	2.46	13	1
1:A:65:LEU:HD23	1:A:69:GLU:HG2	0.40	1.93	17	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	80/95 (84%)	74±1 (93±1%)	4±1 (5±2%)	1±1 (2±1%)	12	54
2	B	3/11 (27%)	1±1 (43±26%)	1±1 (45±24%)	0±0 (12±16%)	1	7
All	All	1660/2120 (78%)	1511 (91%)	113 (7%)	36 (2%)	10	49

All 6 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	25	SER	20
2	B	109	ASN	7
1	A	85	PRO	4
1	A	58	ASP	2
1	A	8	ALA	2
1	A	89	SER	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	70/84 (83%)	60±3 (85±4%)	10±3 (15±4%)	6 45
2	B	4/10 (40%)	3±1 (75±21%)	1±1 (25±21%)	2 25
All	All	1480/1880 (79%)	1255 (85%)	225 (15%)	6 44

All 36 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	21	PHE	20
1	A	44	LYS	15
2	B	112	ARG	13
1	A	28	ASN	13
1	A	16	LYS	12
1	A	67	ARG	9
1	A	23	SER	9
1	A	10	LYS	8
1	A	14	LYS	8
1	A	66	ASP	8
1	A	52	ARG	8
1	A	88	MET	8
1	A	13	ASP	7
1	A	68	ASP	7
1	A	43	SER	7
1	A	47	VAL	6
1	A	18	ASP	6
2	B	111	PHE	6
1	A	32	SER	5
1	A	58	ASP	5
1	A	81	LEU	5
1	A	37	LYS	5
1	A	24	LEU	4
1	A	79	CYS	4
1	A	12	GLU	4
1	A	60	ASP	3
1	A	69	GLU	3
1	A	78	TYR	3
1	A	48	ASP	3
1	A	22	ASP	2
1	A	34	ASP	2
1	A	57	SER	2
1	A	25	SER	2
1	A	61	HIS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	109	ASN	1
1	A	89	SER	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)

Of 1 ligands modelled in this entry, 1 is 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 (i)

No chemical shift data were provided