



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 12:39 PM UTC

PDB ID : 1GKN / pdb_00001gkn
Title : Structure Determination and Rational Mutagenesis reveal binding surface of immune adherence receptor, CR1 (CD35)
Authors : Smith, B.O.; Mallin, R.L.; Krych-Goldberg, M.; Wang, X.; Hauhart, R.E.; Bromek, K.; Uhrin, D.; Atkinson, J.P.; Barlow, P.N.
Deposited on : 2001-08-16

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

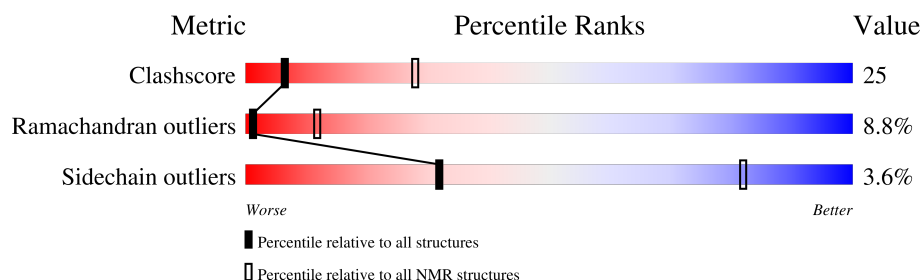
1 Overall quality at a glance

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	128	44% 54% .

2 Ensemble composition and analysis

This entry contains 24 models. Model 3 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:900-A:1024 (125)	1.70	3

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1970 atoms, of which 976 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COMPLEMENT RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			1970	624	976	175	186	9	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	918	THR	ASN	engineered mutation	UNP P17927
A	987	THR	ASN	engineered mutation	UNP P17927

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: COMPLEMENT RECEPTOR TYPE 1

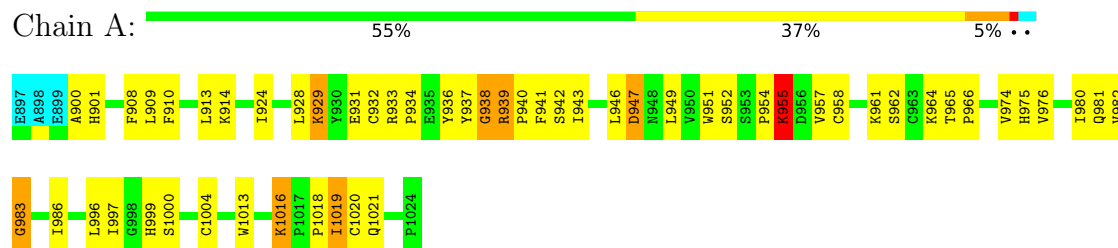


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1



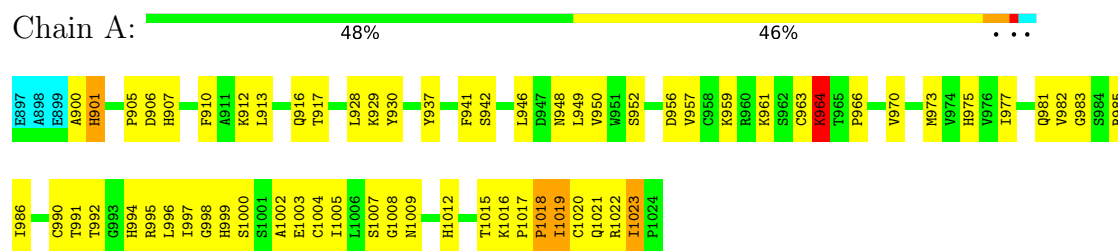
4.2.2 Score per residue for model 2

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1



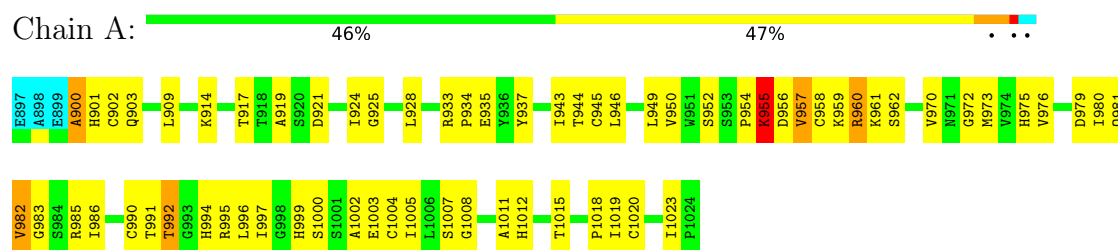
4.2.6 Score per residue for model 6

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1



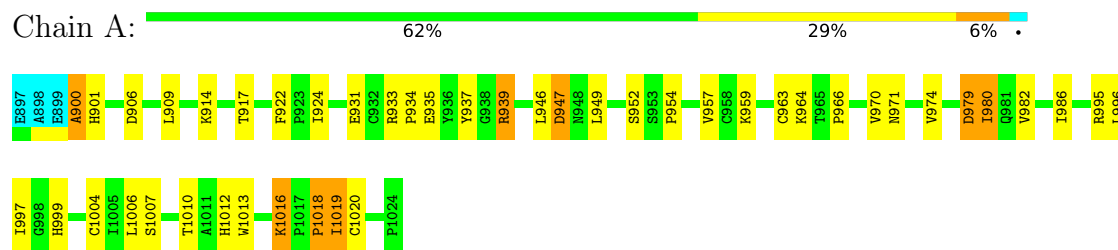
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1



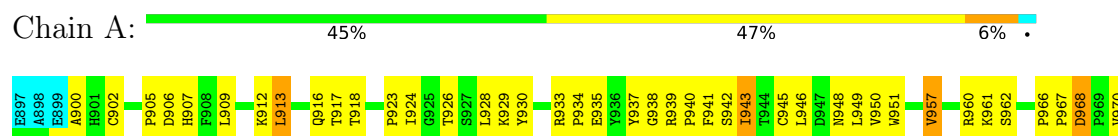
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1



4.2.9 Score per residue for model 9

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

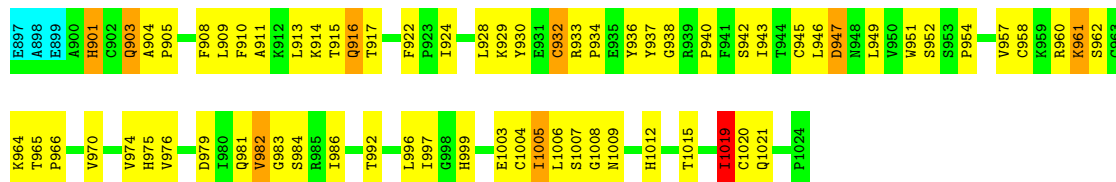




4.2.10 Score per residue for model 10

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

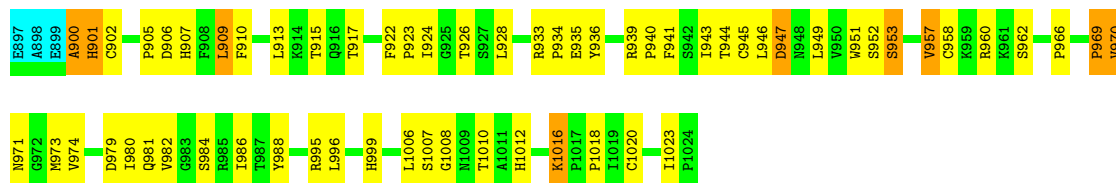
Chain A: 45% 46% 6% ..



4.2.11 Score per residue for model 11

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

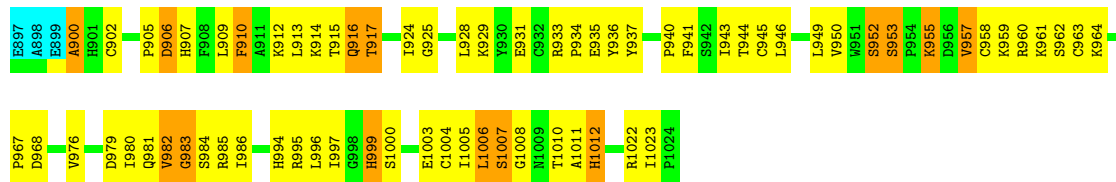
Chain A: 50% 41% 7% .



4.2.12 Score per residue for model 12

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

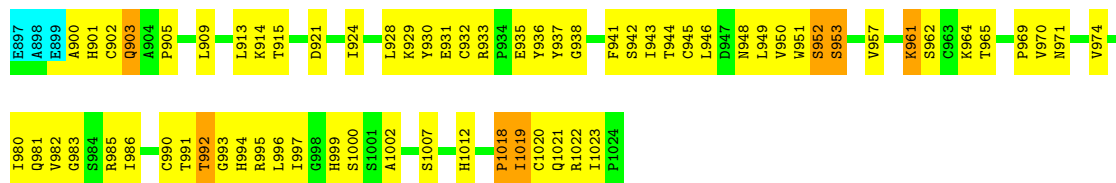
Chain A: 43% 43% 12% .



4.2.13 Score per residue for model 13

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

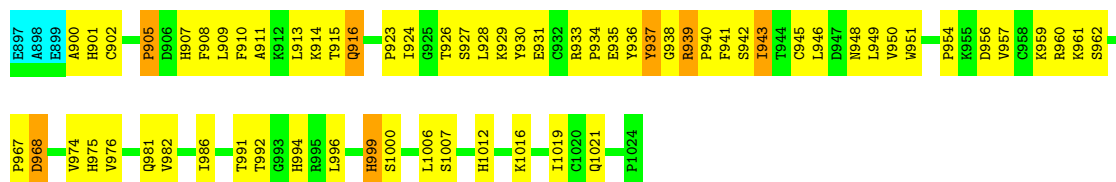
Chain A: 45% 47% 5% .



4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

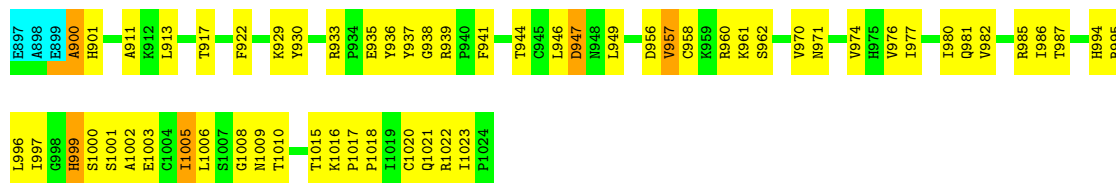
Chain A: 47% 45% 5% •



4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

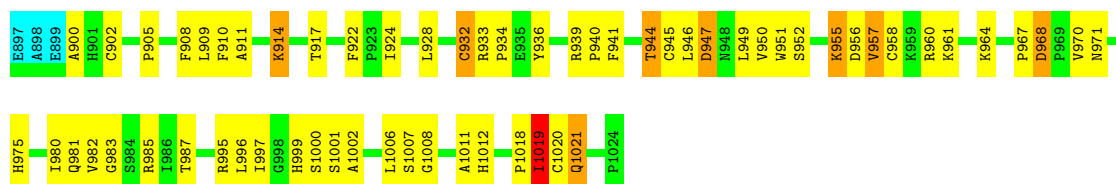
Chain A: 52% 41% • •



4.2.16 Score per residue for model 16

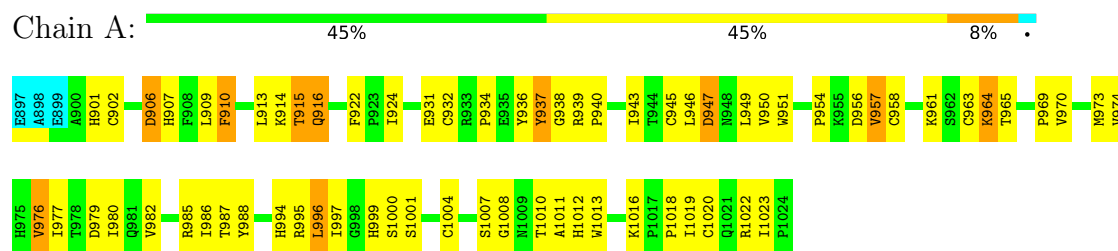
- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A: 50% 41% 6% • •



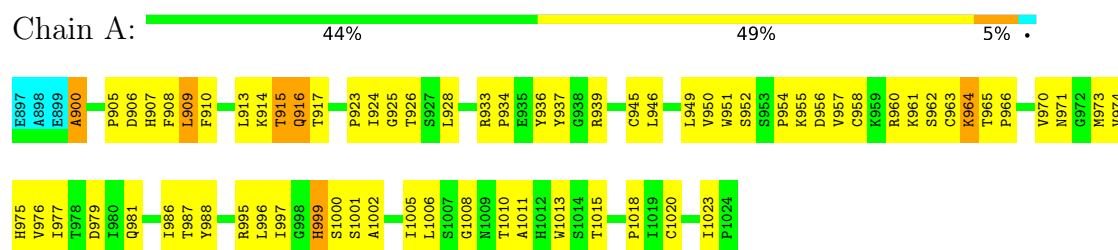
4.2.17 Score per residue for model 17

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1



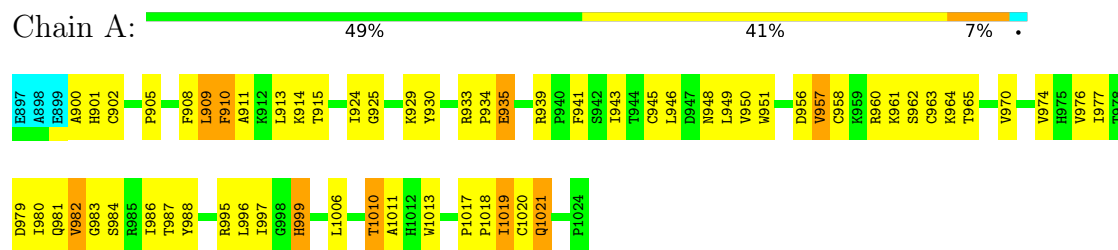
4.2.18 Score per residue for model 18

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1



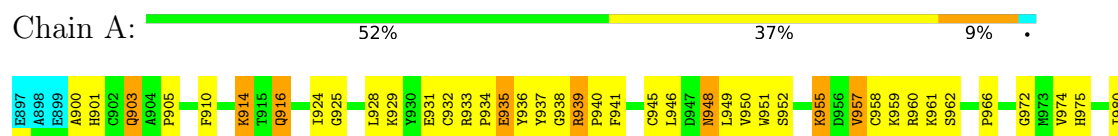
4.2.19 Score per residue for model 19

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1



4.2.20 Score per residue for model 20

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

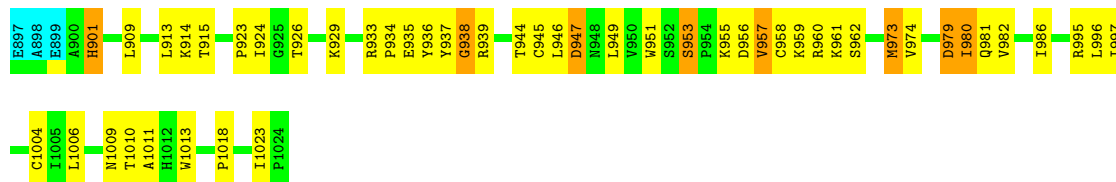




4.2.21 Score per residue for model 21

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

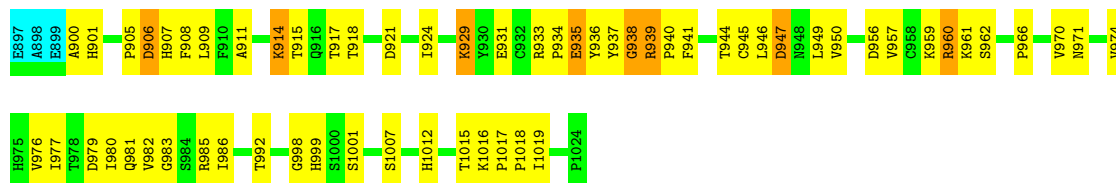
Chain A: 59% 32% 6% .



4.2.22 Score per residue for model 22

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

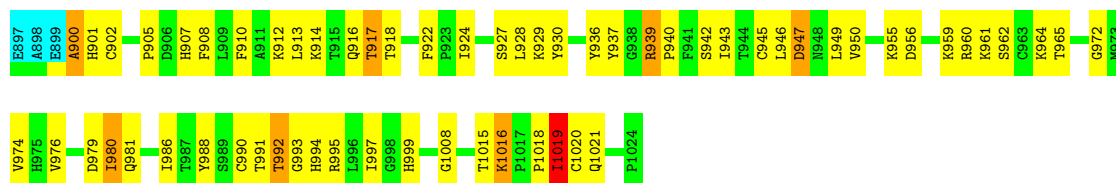
Chain A: 50% 41% 6% .



4.2.23 Score per residue for model 23

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A: 50% 41% 5% ..



4.2.24 Score per residue for model 24

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A: 38% 51% 9% .

Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000	Y1001	Y1002	Y1003	Y1004	Y1005	Y1006	Y1007	Y1008	Y1009	Y1010	Y1011	Y1012	Y1013	Y1014	Y1015	Y1016	Y1017	Y1018	Y1019	Y1020	Y1021	Y1022	Y1023	Y1024
Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000	Y1001	Y1002	Y1003	Y1004	Y1005	Y1006	Y1007	Y1008	Y1009	Y1010	Y1011	Y1012	Y1013	Y1014	Y1015	Y1016	Y1017	Y1018	Y1019	Y1020	Y1021	Y1022	Y1023	Y1024

5 Refinement protocol and experimental data overview

The models were refined using the following method: *MOLECULAR DYNAMICS SIMULATED ANNEALING*.

Of the 120 calculated structures, 24 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	1.0
CNS	structure solution	1.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	971	957	951	49±10
All	All	23304	22968	22824	1166

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:976:VAL:HG13	1:A:980:ILE:HG23	0.94	1.39	22	5
1:A:1007:SER:HA	1:A:1011:ALA:HA	0.87	1.45	24	2
1:A:900:ALA:HB1	1:A:949:LEU:HD21	0.84	1.47	7	11
1:A:935:GLU:HB3	1:A:982:VAL:HG21	0.84	1.50	21	1
1:A:915:THR:HG21	1:A:928:LEU:HD22	0.83	1.47	18	1
1:A:909:LEU:HD12	1:A:910:PHE:N	0.82	1.89	17	1
1:A:1006:LEU:HD13	1:A:1007:SER:N	0.81	1.91	12	2
1:A:938:GLY:HA3	1:A:958:CYS:HA	0.81	1.52	17	4
1:A:900:ALA:HB1	1:A:949:LEU:HD11	0.80	1.50	9	7
1:A:975:HIS:HB3	1:A:987:THR:HG23	0.79	1.53	18	1
1:A:997:ILE:HB	1:A:1019:ILE:HG23	0.78	1.55	8	2
1:A:939:ARG:HB2	1:A:940:PRO:HD2	0.78	1.55	4	8
1:A:974:VAL:HG21	1:A:986:ILE:HD12	0.77	1.57	1	13
1:A:961:LYS:HG3	1:A:962:SER:H	0.76	1.41	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:931:GLU:HG2	1:A:940:PRO:HB3	0.76	1.58	17	3
1:A:946:LEU:HD23	1:A:950:VAL:HG23	0.75	1.58	7	8
1:A:961:LYS:HE3	1:A:1011:ALA:HB2	0.74	1.60	16	1
1:A:997:ILE:HD11	1:A:1021:GLN:HG2	0.74	1.57	24	2
1:A:961:LYS:HD3	1:A:962:SER:N	0.71	1.99	14	1
1:A:902:CYS:HB3	1:A:949:LEU:HA	0.70	1.62	24	4
1:A:997:ILE:HD11	1:A:1021:GLN:HB2	0.70	1.62	23	3
1:A:959:LYS:HA	1:A:959:LYS:HE2	0.70	1.63	12	3
1:A:914:LYS:HA	1:A:914:LYS:HE3	0.69	1.64	16	1
1:A:913:LEU:HD13	1:A:914:LYS:N	0.69	2.03	12	7
1:A:913:LEU:HD11	1:A:928:LEU:HD21	0.69	1.65	9	1
1:A:941:PHE:HB3	1:A:957:VAL:HB	0.69	1.65	14	2
1:A:976:VAL:HA	1:A:986:ILE:HG22	0.68	1.64	12	10
1:A:994:HIS:HA	1:A:1022:ARG:HA	0.68	1.65	12	5
1:A:960:ARG:HE	1:A:981:GLN:HB3	0.68	1.48	10	1
1:A:908:PHE:HB2	1:A:911:ALA:HB3	0.68	1.65	16	1
1:A:927:SER:HB2	1:A:942:SER:HB2	0.68	1.65	14	2
1:A:1019:ILE:HG22	1:A:1020:CYS:H	0.67	1.49	24	8
1:A:914:LYS:HA	1:A:914:LYS:HE2	0.67	1.67	22	1
1:A:946:LEU:HD22	1:A:946:LEU:N	0.67	2.03	14	11
1:A:961:LYS:HG2	1:A:982:VAL:HG13	0.67	1.65	19	1
1:A:924:ILE:HA	1:A:945:CYS:SG	0.67	2.30	22	16
1:A:911:ALA:HB1	1:A:930:TYR:HB3	0.66	1.67	14	1
1:A:924:ILE:HD13	1:A:947:ASP:HA	0.66	1.68	8	9
1:A:960:ARG:HD3	1:A:981:GLN:HB3	0.65	1.67	9	1
1:A:946:LEU:HD21	1:A:952:SER:N	0.65	2.07	7	3
1:A:960:ARG:HD2	1:A:981:GLN:HB3	0.65	1.69	2	5
1:A:935:GLU:O	1:A:961:LYS:HD2	0.65	1.92	19	1
1:A:961:LYS:HD3	1:A:1011:ALA:HB2	0.65	1.68	18	2
1:A:914:LYS:HG3	1:A:931:GLU:HG2	0.64	1.70	12	1
1:A:909:LEU:HD22	1:A:909:LEU:N	0.64	2.07	11	6
1:A:961:LYS:HG3	1:A:962:SER:N	0.64	2.07	12	1
1:A:929:LYS:HD3	1:A:942:SER:HB3	0.64	1.69	23	1
1:A:943:ILE:HB	1:A:951:TRP:HB3	0.64	1.70	10	5
1:A:961:LYS:HG2	1:A:1007:SER:HB2	0.64	1.67	12	1
1:A:972:GLY:HA2	1:A:991:THR:H	0.64	1.53	7	1
1:A:909:LEU:O	1:A:933:ARG:HD3	0.63	1.93	12	4
1:A:970:VAL:HB	1:A:1020:CYS:HB2	0.63	1.70	11	1
1:A:991:THR:HG22	1:A:1020:CYS:SG	0.63	2.32	13	1
1:A:908:PHE:HB3	1:A:911:ALA:HB3	0.63	1.69	24	2
1:A:924:ILE:HD13	1:A:945:CYS:SG	0.63	2.34	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:990:CYS:SG	1:A:994:HIS:HB2	0.63	2.34	7	1
1:A:961:LYS:HD3	1:A:1007:SER:HB2	0.62	1.71	24	1
1:A:960:ARG:HB3	1:A:981:GLN:NE2	0.62	2.09	2	3
1:A:913:LEU:HD11	1:A:915:THR:O	0.62	1.94	21	4
1:A:975:HIS:NE2	1:A:977:ILE:HG13	0.62	2.09	3	1
1:A:965:THR:HA	1:A:980:ILE:HD12	0.62	1.68	19	5
1:A:960:ARG:HD2	1:A:961:LYS:NZ	0.62	2.09	19	1
1:A:939:ARG:HD3	1:A:939:ARG:H	0.62	1.55	8	1
1:A:962:SER:HB3	1:A:981:GLN:NE2	0.61	2.10	24	10
1:A:924:ILE:HD11	1:A:949:LEU:HD23	0.61	1.71	2	1
1:A:966:PRO:HG2	1:A:974:VAL:HG11	0.61	1.71	9	4
1:A:982:VAL:HG13	1:A:1005:ILE:HA	0.61	1.71	24	4
1:A:996:LEU:HD23	1:A:997:ILE:N	0.61	2.11	3	8
1:A:964:LYS:HE3	1:A:964:LYS:HA	0.61	1.71	4	1
1:A:929:LYS:HA	1:A:942:SER:HA	0.61	1.72	9	2
1:A:957:VAL:HG23	1:A:958:CYS:H	0.60	1.56	15	6
1:A:962:SER:HB3	1:A:981:GLN:HE21	0.60	1.56	11	4
1:A:924:ILE:HG21	1:A:947:ASP:HA	0.60	1.73	3	7
1:A:999:HIS:ND1	1:A:1015:THR:HG21	0.60	2.11	23	2
1:A:1006:LEU:HD12	1:A:1010:THR:C	0.60	2.21	18	4
1:A:937:TYR:HD2	1:A:961:LYS:HA	0.60	1.55	18	5
1:A:946:LEU:HB2	1:A:950:VAL:CG2	0.60	2.27	9	11
1:A:959:LYS:H	1:A:959:LYS:HD2	0.60	1.56	8	1
1:A:913:LEU:HD12	1:A:929:LYS:O	0.59	1.98	5	1
1:A:936:TYR:HA	1:A:960:ARG:HA	0.59	1.74	21	3
1:A:996:LEU:HD13	1:A:997:ILE:N	0.59	2.13	7	3
1:A:961:LYS:HB2	1:A:961:LYS:NZ	0.59	2.13	10	2
1:A:1007:SER:CA	1:A:1011:ALA:HA	0.59	2.27	24	1
1:A:913:LEU:HD21	1:A:915:THR:HG22	0.59	1.74	18	1
1:A:914:LYS:HD3	1:A:929:LYS:HG2	0.59	1.73	19	1
1:A:1006:LEU:HD12	1:A:1011:ALA:HB2	0.59	1.73	19	1
1:A:956:ASP:HA	1:A:959:LYS:HE2	0.59	1.75	14	3
1:A:985:ARG:HA	1:A:1003:GLU:HA	0.59	1.75	12	4
1:A:972:GLY:HA3	1:A:1020:CYS:SG	0.59	2.37	5	2
1:A:977:ILE:HG22	1:A:978:THR:HG23	0.58	1.74	3	1
1:A:956:ASP:HA	1:A:959:LYS:HE3	0.58	1.75	23	1
1:A:1005:ILE:O	1:A:1006:LEU:O	0.58	2.20	12	1
1:A:909:LEU:HD22	1:A:910:PHE:N	0.58	2.12	19	1
1:A:937:TYR:CD2	1:A:961:LYS:HA	0.58	2.34	18	13
1:A:916:GLN:NE2	1:A:916:GLN:H	0.58	1.96	10	3
1:A:999:HIS:ND1	1:A:1015:THR:HB	0.58	2.13	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:908:PHE:O	1:A:909:LEU:HD13	0.58	1.97	18	1
1:A:995:ARG:HB3	1:A:1023:ILE:HG12	0.58	1.76	11	11
1:A:999:HIS:O	1:A:1018:PRO:HG3	0.58	1.98	11	3
1:A:917:THR:HB	1:A:922:PHE:HZ	0.58	1.59	16	2
1:A:962:SER:HB2	1:A:981:GLN:HG3	0.58	1.75	23	1
1:A:944:THR:O	1:A:946:LEU:HD22	0.58	1.99	12	4
1:A:909:LEU:O	1:A:933:ARG:HD2	0.57	1.98	11	7
1:A:960:ARG:HD2	1:A:981:GLN:HB2	0.57	1.76	18	1
1:A:998:GLY:HA3	1:A:1018:PRO:HB3	0.57	1.76	6	2
1:A:955:LYS:HD3	1:A:956:ASP:N	0.57	2.14	21	2
1:A:929:LYS:HD2	1:A:940:PRO:HB2	0.57	1.76	3	2
1:A:962:SER:HB3	1:A:981:GLN:HE22	0.57	1.60	4	1
1:A:937:TYR:HB3	1:A:961:LYS:HD2	0.57	1.76	24	1
1:A:937:TYR:HB3	1:A:961:LYS:HZ3	0.57	1.59	12	1
1:A:913:LEU:HD11	1:A:915:THR:HG22	0.57	1.75	18	1
1:A:996:LEU:C	1:A:997:ILE:HD12	0.57	2.25	1	1
1:A:961:LYS:CG	1:A:982:VAL:HG22	0.57	2.30	19	1
1:A:955:LYS:HB2	1:A:955:LYS:NZ	0.57	2.15	7	3
1:A:977:ILE:HD12	1:A:985:ARG:O	0.56	2.00	5	2
1:A:911:ALA:HB2	1:A:958:CYS:SG	0.56	2.40	15	2
1:A:995:ARG:O	1:A:997:ILE:HD12	0.56	1.99	9	14
1:A:982:VAL:HA	1:A:1004:CYS:SG	0.56	2.40	17	5
1:A:901:HIS:C	1:A:949:LEU:HD22	0.56	2.26	20	5
1:A:1006:LEU:HD13	1:A:1006:LEU:C	0.56	2.24	12	2
1:A:909:LEU:HD13	1:A:909:LEU:N	0.56	2.15	19	1
1:A:941:PHE:HB3	1:A:957:VAL:HG11	0.56	1.77	3	2
1:A:985:ARG:HG2	1:A:1003:GLU:HB2	0.56	1.77	7	1
1:A:964:LYS:HD3	1:A:965:THR:N	0.56	2.16	1	2
1:A:1007:SER:HB2	1:A:1012:HIS:NE2	0.56	2.16	11	10
1:A:991:THR:O	1:A:992:THR:C	0.56	2.49	24	3
1:A:977:ILE:HD11	1:A:987:THR:HG22	0.56	1.78	18	1
1:A:976:VAL:HB	1:A:979:ASP:O	0.56	2.01	3	4
1:A:1007:SER:HA	1:A:1011:ALA:CA	0.56	2.26	24	1
1:A:948:ASN:O	1:A:950:VAL:HG13	0.55	2.01	5	7
1:A:948:ASN:HD22	1:A:948:ASN:N	0.55	1.99	20	1
1:A:946:LEU:HD21	1:A:952:SER:H	0.55	1.59	7	1
1:A:1016:LYS:O	1:A:1016:LYS:HD3	0.55	2.01	24	1
1:A:929:LYS:NZ	1:A:929:LYS:HB2	0.55	2.16	1	2
1:A:914:LYS:HD2	1:A:931:GLU:HG3	0.55	1.76	3	1
1:A:1010:THR:HG22	1:A:1011:ALA:H	0.55	1.62	19	1
1:A:970:VAL:O	1:A:1020:CYS:HB2	0.55	2.02	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:939:ARG:HD2	1:A:939:ARG:H	0.55	1.61	5	1
1:A:931:GLU:OE1	1:A:940:PRO:HB3	0.55	2.02	5	2
1:A:914:LYS:HB2	1:A:931:GLU:HG2	0.55	1.79	14	2
1:A:991:THR:O	1:A:992:THR:CB	0.55	2.55	20	1
1:A:914:LYS:O	1:A:915:THR:C	0.55	2.50	5	1
1:A:1016:LYS:NZ	1:A:1016:LYS:HB3	0.55	2.17	11	1
1:A:1007:SER:HA	1:A:1010:THR:O	0.55	2.01	12	2
1:A:909:LEU:HD12	1:A:909:LEU:C	0.55	2.26	17	1
1:A:962:SER:HA	1:A:981:GLN:HA	0.55	1.78	18	3
1:A:936:TYR:HA	1:A:961:LYS:H	0.55	1.61	18	2
1:A:975:HIS:O	1:A:977:ILE:HD12	0.55	2.02	3	1
1:A:1007:SER:HB3	1:A:1012:HIS:NE2	0.55	2.17	9	2
1:A:957:VAL:HG23	1:A:958:CYS:N	0.54	2.17	1	5
1:A:997:ILE:HB	1:A:1019:ILE:HB	0.54	1.77	17	5
1:A:1006:LEU:HB3	1:A:1012:HIS:NE2	0.54	2.16	12	2
1:A:928:LEU:N	1:A:942:SER:O	0.54	2.40	3	2
1:A:913:LEU:HD22	1:A:914:LYS:H	0.54	1.63	10	1
1:A:955:LYS:NZ	1:A:955:LYS:HB3	0.54	2.18	24	1
1:A:939:ARG:HD2	1:A:939:ARG:C	0.54	2.27	24	3
1:A:928:LEU:O	1:A:943:ILE:HG12	0.54	2.02	9	1
1:A:922:PHE:CE2	1:A:928:LEU:HD11	0.54	2.38	10	2
1:A:908:PHE:C	1:A:909:LEU:HD13	0.54	2.28	18	1
1:A:934:PRO:O	1:A:935:GLU:HG3	0.54	2.02	4	5
1:A:901:HIS:N	1:A:949:LEU:HD22	0.54	2.17	6	4
1:A:928:LEU:HD23	1:A:930:TYR:OH	0.54	2.03	14	1
1:A:961:LYS:NZ	1:A:1006:LEU:HD11	0.54	2.18	3	1
1:A:995:ARG:HB3	1:A:1021:GLN:O	0.54	2.02	23	1
1:A:909:LEU:N	1:A:909:LEU:CD1	0.54	2.71	19	4
1:A:902:CYS:SG	1:A:949:LEU:HA	0.53	2.43	12	6
1:A:901:HIS:O	1:A:949:LEU:HG	0.53	2.03	1	4
1:A:960:ARG:NE	1:A:981:GLN:HB3	0.53	2.18	10	2
1:A:929:LYS:HD3	1:A:941:PHE:O	0.53	2.03	12	4
1:A:909:LEU:N	1:A:909:LEU:HD12	0.53	2.18	3	5
1:A:916:GLN:H	1:A:916:GLN:CD	0.53	2.11	9	1
1:A:970:VAL:HG22	1:A:971:ASN:ND2	0.53	2.19	18	7
1:A:1006:LEU:HG	1:A:1008:GLY:H	0.53	1.63	11	1
1:A:912:LYS:HE2	1:A:933:ARG:NE	0.53	2.18	12	1
1:A:975:HIS:CD2	1:A:977:ILE:HG12	0.53	2.39	5	1
1:A:945:CYS:HA	1:A:950:VAL:O	0.53	2.03	16	6
1:A:914:LYS:HG3	1:A:931:GLU:HG3	0.53	1.81	20	2
1:A:909:LEU:HD22	1:A:909:LEU:C	0.53	2.28	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:913:LEU:HD13	1:A:913:LEU:C	0.53	2.29	18	6
1:A:929:LYS:HG2	1:A:942:SER:HB3	0.53	1.81	10	1
1:A:913:LEU:HD22	1:A:915:THR:O	0.53	2.03	13	2
1:A:948:ASN:ND2	1:A:950:VAL:HG22	0.53	2.18	20	1
1:A:924:ILE:HG12	1:A:945:CYS:SG	0.53	2.44	16	2
1:A:911:ALA:HA	1:A:932:CYS:HA	0.53	1.79	16	3
1:A:962:SER:HB3	1:A:981:GLN:OE1	0.53	2.04	9	1
1:A:935:GLU:C	1:A:961:LYS:HB3	0.53	2.29	19	1
1:A:914:LYS:HB3	1:A:914:LYS:NZ	0.53	2.18	20	2
1:A:967:PRO:O	1:A:968:ASP:C	0.52	2.52	12	5
1:A:917:THR:HG21	1:A:928:LEU:HD11	0.52	1.81	5	2
1:A:963:CYS:HA	1:A:1011:ALA:HB1	0.52	1.82	12	1
1:A:981:GLN:O	1:A:1004:CYS:HB3	0.52	2.04	9	4
1:A:979:ASP:HB3	1:A:981:GLN:OE1	0.52	2.04	11	3
1:A:994:HIS:HB2	1:A:1020:CYS:SG	0.52	2.44	23	2
1:A:912:LYS:HB2	1:A:912:LYS:NZ	0.52	2.20	6	1
1:A:913:LEU:HD21	1:A:917:THR:HG23	0.52	1.82	11	1
1:A:936:TYR:C	1:A:961:LYS:HE2	0.52	2.30	12	1
1:A:913:LEU:C	1:A:913:LEU:HD13	0.52	2.29	17	4
1:A:901:HIS:C	1:A:949:LEU:HD12	0.52	2.30	17	2
1:A:979:ASP:O	1:A:980:ILE:HG12	0.52	2.05	17	2
1:A:902:CYS:O	1:A:922:PHE:HB2	0.52	2.05	11	5
1:A:976:VAL:O	1:A:977:ILE:HB	0.52	2.04	3	1
1:A:1021:GLN:C	1:A:1023:ILE:H	0.52	2.12	6	1
1:A:948:ASN:ND2	1:A:948:ASN:H	0.52	2.03	20	1
1:A:982:VAL:HG21	1:A:1007:SER:OG	0.52	2.05	24	1
1:A:946:LEU:O	1:A:947:ASP:HB2	0.51	2.05	8	14
1:A:937:TYR:HB3	1:A:961:LYS:NZ	0.51	2.20	21	2
1:A:935:GLU:C	1:A:961:LYS:HD3	0.51	2.29	21	1
1:A:934:PRO:O	1:A:935:GLU:HB2	0.51	2.05	21	6
1:A:1006:LEU:HD12	1:A:1012:HIS:NE2	0.51	2.20	12	1
1:A:981:GLN:C	1:A:983:GLY:H	0.51	2.14	9	3
1:A:996:LEU:HD13	1:A:996:LEU:C	0.51	2.30	19	2
1:A:943:ILE:HD12	1:A:951:TRP:CE3	0.51	2.40	17	1
1:A:961:LYS:CE	1:A:982:VAL:HG22	0.51	2.35	19	1
1:A:931:GLU:HA	1:A:940:PRO:HB3	0.51	1.80	22	1
1:A:938:GLY:O	1:A:939:ARG:O	0.51	2.29	20	6
1:A:927:SER:HB3	1:A:944:THR:OG1	0.51	2.06	3	1
1:A:986:ILE:O	1:A:986:ILE:HG13	0.51	2.06	18	4
1:A:979:ASP:O	1:A:984:SER:HB2	0.51	2.05	12	2
1:A:995:ARG:HH21	1:A:1023:ILE:HG23	0.51	1.65	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:905:PRO:HG3	1:A:928:LEU:HD12	0.51	1.82	20	1
1:A:972:GLY:HA2	1:A:990:CYS:HA	0.51	1.80	4	3
1:A:985:ARG:HG3	1:A:1002:ALA:C	0.51	2.31	15	3
1:A:963:CYS:SG	1:A:1013:TRP:CE2	0.51	3.04	8	2
1:A:905:PRO:HG3	1:A:951:TRP:CE2	0.51	2.41	24	2
1:A:915:THR:HG22	1:A:916:GLN:NE2	0.51	2.20	24	1
1:A:905:PRO:HG2	1:A:928:LEU:HD23	0.51	1.83	16	1
1:A:996:LEU:HD23	1:A:996:LEU:C	0.51	2.31	2	13
1:A:914:LYS:HD2	1:A:914:LYS:C	0.51	2.31	21	4
1:A:974:VAL:O	1:A:974:VAL:HG13	0.51	2.06	21	1
1:A:1016:LYS:N	1:A:1016:LYS:HD3	0.50	2.21	14	1
1:A:961:LYS:HE3	1:A:1008:GLY:H	0.50	1.66	12	1
1:A:977:ILE:HD13	1:A:985:ARG:O	0.50	2.06	3	2
1:A:998:GLY:O	1:A:1018:PRO:HB3	0.50	2.06	5	1
1:A:935:GLU:HB3	1:A:982:VAL:HG11	0.50	1.82	12	1
1:A:981:GLN:O	1:A:983:GLY:N	0.50	2.45	10	9
1:A:927:SER:HB2	1:A:942:SER:OG	0.50	2.06	4	1
1:A:956:ASP:OD1	1:A:959:LYS:HE2	0.50	2.07	7	1
1:A:960:ARG:HG3	1:A:981:GLN:NE2	0.50	2.21	22	1
1:A:997:ILE:CD1	1:A:1021:GLN:HG2	0.50	2.37	1	1
1:A:1002:ALA:HB2	1:A:1015:THR:OG1	0.50	2.06	6	3
1:A:951:TRP:C	1:A:953:SER:N	0.50	2.70	21	1
1:A:946:LEU:N	1:A:946:LEU:CD2	0.50	2.75	14	7
1:A:961:LYS:HG2	1:A:1007:SER:CB	0.50	2.35	12	1
1:A:908:PHE:O	1:A:909:LEU:HB2	0.50	2.06	1	4
1:A:960:ARG:HD3	1:A:961:LYS:N	0.50	2.21	2	1
1:A:937:TYR:HD2	1:A:961:LYS:HD2	0.50	1.67	15	1
1:A:955:LYS:N	1:A:955:LYS:HD3	0.49	2.22	12	1
1:A:910:PHE:HA	1:A:933:ARG:HD2	0.49	1.84	14	2
1:A:997:ILE:HD13	1:A:1021:GLN:HB2	0.49	1.84	19	1
1:A:1016:LYS:HD2	1:A:1017:PRO:N	0.49	2.22	6	2
1:A:960:ARG:CG	1:A:981:GLN:HB3	0.49	2.37	12	1
1:A:995:ARG:HB2	1:A:1023:ILE:HG12	0.49	1.82	24	1
1:A:905:PRO:O	1:A:906:ASP:C	0.49	2.56	22	5
1:A:987:THR:HA	1:A:1001:SER:HA	0.49	1.83	18	1
1:A:913:LEU:HD13	1:A:930:TYR:CE1	0.49	2.43	15	1
1:A:916:GLN:O	1:A:917:THR:HG22	0.49	2.07	12	1
1:A:903:GLN:H	1:A:903:GLN:CD	0.49	2.16	20	2
1:A:903:GLN:H	1:A:903:GLN:NE2	0.49	2.05	20	2
1:A:962:SER:HB3	1:A:981:GLN:HG3	0.49	1.84	13	1
1:A:1005:ILE:H	1:A:1005:ILE:HD13	0.49	1.68	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:930:TYR:O	1:A:940:PRO:HB3	0.49	2.08	3	1
1:A:996:LEU:HD22	1:A:999:HIS:O	0.49	2.08	14	1
1:A:985:ARG:HD3	1:A:1001:SER:HB2	0.49	1.84	22	1
1:A:916:GLN:CD	1:A:917:THR:N	0.49	2.70	23	1
1:A:964:LYS:HB3	1:A:964:LYS:NZ	0.49	2.22	6	1
1:A:991:THR:O	1:A:992:THR:HB	0.49	2.08	20	3
1:A:977:ILE:HD12	1:A:977:ILE:N	0.49	2.22	17	1
1:A:1016:LYS:O	1:A:1016:LYS:HD2	0.49	2.08	23	3
1:A:1019:ILE:HD12	1:A:1019:ILE:H	0.49	1.67	19	1
1:A:906:ASP:CG	1:A:907:HIS:H	0.49	2.16	9	3
1:A:916:GLN:O	1:A:917:THR:O	0.49	2.31	23	2
1:A:906:ASP:CG	1:A:907:HIS:N	0.48	2.71	5	2
1:A:977:ILE:HD11	1:A:987:THR:OG1	0.48	2.08	19	2
1:A:957:VAL:HG12	1:A:958:CYS:N	0.48	2.23	20	1
1:A:951:TRP:O	1:A:952:SER:C	0.48	2.56	4	4
1:A:923:PRO:HG2	1:A:926:THR:OG1	0.48	2.08	24	7
1:A:930:TYR:CE1	1:A:943:ILE:HD11	0.48	2.42	3	1
1:A:996:LEU:HD21	1:A:1018:PRO:HB2	0.48	1.83	13	1
1:A:910:PHE:O	1:A:933:ARG:HG3	0.48	2.08	24	1
1:A:967:PRO:O	1:A:968:ASP:O	0.48	2.31	9	2
1:A:946:LEU:HD11	1:A:952:SER:HA	0.48	1.85	16	1
1:A:914:LYS:HE2	1:A:929:LYS:HD2	0.48	1.84	21	1
1:A:996:LEU:C	1:A:996:LEU:HD13	0.48	2.34	10	1
1:A:996:LEU:HD21	1:A:1018:PRO:HB3	0.48	1.85	24	2
1:A:960:ARG:HD2	1:A:982:VAL:HB	0.48	1.85	24	1
1:A:928:LEU:HD23	1:A:930:TYR:CE1	0.48	2.44	5	1
1:A:961:LYS:CD	1:A:1007:SER:HB2	0.48	2.39	24	1
1:A:1016:LYS:HD2	1:A:1016:LYS:C	0.48	2.33	8	6
1:A:994:HIS:HA	1:A:1021:GLN:O	0.48	2.09	6	1
1:A:1021:GLN:O	1:A:1022:ARG:C	0.48	2.56	24	1
1:A:948:ASN:N	1:A:948:ASN:ND2	0.48	2.61	20	1
1:A:955:LYS:HD3	1:A:955:LYS:C	0.48	2.34	23	1
1:A:1005:ILE:HD13	1:A:1005:ILE:N	0.48	2.24	2	1
1:A:975:HIS:NE2	1:A:977:ILE:HG12	0.48	2.24	5	1
1:A:912:LYS:HB3	1:A:933:ARG:CZ	0.48	2.39	9	1
1:A:1006:LEU:HD12	1:A:1011:ALA:N	0.48	2.24	21	2
1:A:952:SER:O	1:A:953:SER:O	0.47	2.32	13	2
1:A:961:LYS:HB2	1:A:961:LYS:HZ3	0.47	1.68	10	1
1:A:1006:LEU:C	1:A:1006:LEU:HD23	0.47	2.34	10	1
1:A:906:ASP:O	1:A:907:HIS:C	0.47	2.57	4	1
1:A:946:LEU:HB2	1:A:950:VAL:HG23	0.47	1.85	24	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:979:ASP:CG	1:A:980:ILE:H	0.47	2.18	8	3
1:A:951:TRP:O	1:A:954:PRO:HD3	0.47	2.09	17	1
1:A:987:THR:OG1	1:A:988:TYR:N	0.47	2.47	18	1
1:A:913:LEU:HD21	1:A:917:THR:OG1	0.47	2.09	6	1
1:A:910:PHE:O	1:A:932:CYS:HA	0.47	2.10	17	4
1:A:936:TYR:CD2	1:A:960:ARG:HA	0.47	2.45	2	2
1:A:912:LYS:HG3	1:A:933:ARG:HD2	0.47	1.85	12	1
1:A:996:LEU:O	1:A:996:LEU:HD12	0.47	2.09	1	1
1:A:988:TYR:CD2	1:A:1018:PRO:HD2	0.47	2.45	2	3
1:A:933:ARG:HB3	1:A:934:PRO:HD2	0.47	1.86	19	3
1:A:937:TYR:O	1:A:958:CYS:HA	0.47	2.10	4	1
1:A:900:ALA:HA	1:A:949:LEU:HD11	0.47	1.85	6	2
1:A:901:HIS:C	1:A:949:LEU:HG	0.47	2.34	8	2
1:A:905:PRO:HG3	1:A:951:TRP:CZ2	0.47	2.44	10	2
1:A:991:THR:O	1:A:993:GLY:N	0.47	2.48	9	1
1:A:924:ILE:HA	1:A:945:CYS:HB3	0.47	1.85	21	2
1:A:961:LYS:HG3	1:A:982:VAL:HG22	0.47	1.86	19	1
1:A:908:PHE:CB	1:A:911:ALA:HB3	0.47	2.39	24	2
1:A:930:TYR:HB2	1:A:941:PHE:CZ	0.47	2.44	5	2
1:A:963:CYS:O	1:A:964:LYS:O	0.47	2.33	17	3
1:A:951:TRP:C	1:A:953:SER:H	0.47	2.18	21	2
1:A:915:THR:O	1:A:917:THR:HG23	0.47	2.09	2	3
1:A:929:LYS:HG3	1:A:941:PHE:O	0.47	2.10	20	4
1:A:976:VAL:HG13	1:A:979:ASP:O	0.47	2.10	18	2
1:A:914:LYS:O	1:A:914:LYS:HD2	0.47	2.09	23	1
1:A:916:GLN:NE2	1:A:917:THR:H	0.46	2.07	23	1
1:A:943:ILE:CG2	1:A:954:PRO:HG3	0.46	2.40	7	1
1:A:957:VAL:CG1	1:A:958:CYS:N	0.46	2.79	20	1
1:A:979:ASP:HB2	1:A:981:GLN:OE1	0.46	2.10	24	2
1:A:934:PRO:C	1:A:936:TYR:H	0.46	2.18	11	7
1:A:966:PRO:HG3	1:A:986:ILE:CD1	0.46	2.41	10	6
1:A:911:ALA:C	1:A:912:LYS:HD3	0.46	2.35	3	1
1:A:957:VAL:HG23	1:A:957:VAL:O	0.46	2.10	11	1
1:A:961:LYS:HD3	1:A:962:SER:H	0.46	1.69	14	1
1:A:948:ASN:HD22	1:A:948:ASN:H	0.46	1.52	20	1
1:A:1016:LYS:C	1:A:1016:LYS:HD3	0.46	2.36	22	2
1:A:939:ARG:HB3	1:A:940:PRO:HD2	0.46	1.88	9	1
1:A:974:VAL:HA	1:A:988:TYR:HA	0.46	1.87	17	1
1:A:901:HIS:HB3	1:A:921:ASP:OD1	0.46	2.09	22	1
1:A:909:LEU:N	1:A:909:LEU:CD2	0.46	2.78	11	6
1:A:925:GLY:O	1:A:944:THR:HG23	0.46	2.10	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:941:PHE:CD2	1:A:957:VAL:HB	0.46	2.46	11	1
1:A:956:ASP:HA	1:A:959:LYS:NZ	0.46	2.25	22	1
1:A:961:LYS:CD	1:A:1011:ALA:HB2	0.46	2.41	7	2
1:A:988:TYR:CE2	1:A:1018:PRO:HD2	0.46	2.46	23	2
1:A:970:VAL:HG12	1:A:971:ASN:H	0.46	1.70	11	1
1:A:900:ALA:HB1	1:A:949:LEU:CD1	0.46	2.41	14	1
1:A:935:GLU:O	1:A:960:ARG:HA	0.46	2.11	15	1
1:A:990:CYS:SG	1:A:996:LEU:HA	0.46	2.51	6	1
1:A:939:ARG:HB2	1:A:940:PRO:CD	0.45	2.37	4	2
1:A:935:GLU:C	1:A:961:LYS:HG3	0.45	2.36	9	1
1:A:908:PHE:CZ	1:A:954:PRO:HG2	0.45	2.46	14	1
1:A:915:THR:HG22	1:A:916:GLN:N	0.45	2.27	17	2
1:A:939:ARG:HD2	1:A:939:ARG:N	0.45	2.26	5	2
1:A:935:GLU:HG3	1:A:936:TYR:CE1	0.45	2.45	15	1
1:A:961:LYS:HZ1	1:A:1011:ALA:H	0.45	1.53	17	1
1:A:961:LYS:O	1:A:981:GLN:HB2	0.45	2.10	18	1
1:A:936:TYR:HA	1:A:959:LYS:O	0.45	2.11	22	1
1:A:905:PRO:HB3	1:A:951:TRP:CG	0.45	2.47	3	1
1:A:913:LEU:HG	1:A:930:TYR:CZ	0.45	2.47	9	2
1:A:937:TYR:CD2	1:A:961:LYS:HD2	0.45	2.47	17	1
1:A:916:GLN:N	1:A:916:GLN:OE1	0.45	2.49	18	1
1:A:910:PHE:C	1:A:933:ARG:HG3	0.45	2.36	20	1
1:A:906:ASP:OD1	1:A:907:HIS:N	0.45	2.50	6	4
1:A:1016:LYS:HD2	1:A:1016:LYS:O	0.45	2.11	9	2
1:A:997:ILE:HD11	1:A:1021:GLN:CG	0.45	2.41	6	1
1:A:914:LYS:O	1:A:929:LYS:HB3	0.45	2.12	1	1
1:A:992:THR:HG22	1:A:993:GLY:N	0.45	2.27	13	1
1:A:905:PRO:HB2	1:A:908:PHE:CD1	0.45	2.47	19	1
1:A:961:LYS:HE3	1:A:982:VAL:HG22	0.45	1.89	19	1
1:A:943:ILE:HG22	1:A:954:PRO:HG3	0.45	1.88	7	1
1:A:957:VAL:O	1:A:958:CYS:HB2	0.45	2.12	11	1
1:A:933:ARG:HB2	1:A:936:TYR:CD1	0.45	2.46	15	3
1:A:914:LYS:HE3	1:A:931:GLU:OE1	0.45	2.12	17	1
1:A:964:LYS:HD3	1:A:964:LYS:C	0.45	2.37	18	1
1:A:918:THR:HG22	1:A:918:THR:O	0.45	2.12	23	1
1:A:979:ASP:OD2	1:A:981:GLN:HB2	0.45	2.12	12	1
1:A:996:LEU:HD21	1:A:1018:PRO:CB	0.45	2.42	13	1
1:A:961:LYS:HZ1	1:A:1006:LEU:HG	0.45	1.72	16	1
1:A:980:ILE:HG22	1:A:986:ILE:CG2	0.45	2.42	17	1
1:A:985:ARG:HG3	1:A:1002:ALA:O	0.44	2.12	16	1
1:A:1005:ILE:O	1:A:1011:ALA:HA	0.44	2.11	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:917:THR:CG2	1:A:928:LEU:HD11	0.44	2.42	2	1
1:A:914:LYS:HD3	1:A:914:LYS:C	0.44	2.37	7	2
1:A:973:MET:HE3	1:A:975:HIS:HE1	0.44	1.71	7	1
1:A:905:PRO:HB3	1:A:943:ILE:HD11	0.44	1.89	12	1
1:A:987:THR:HG22	1:A:1001:SER:HB3	0.44	1.89	17	2
1:A:966:PRO:HG3	1:A:986:ILE:HD11	0.44	1.89	18	1
1:A:944:THR:O	1:A:951:TRP:HA	0.44	2.13	16	1
1:A:928:LEU:O	1:A:942:SER:HA	0.44	2.11	23	5
1:A:974:VAL:CG2	1:A:986:ILE:HB	0.44	2.42	22	4
1:A:985:ARG:HG2	1:A:986:ILE:N	0.44	2.26	17	1
1:A:979:ASP:HB3	1:A:981:GLN:HG2	0.44	1.88	19	1
1:A:973:MET:SD	1:A:973:MET:N	0.44	2.91	21	3
1:A:996:LEU:HA	1:A:1019:ILE:O	0.44	2.13	1	1
1:A:913:LEU:CD2	1:A:928:LEU:HB3	0.44	2.43	12	1
1:A:962:SER:C	1:A:1004:CYS:SG	0.44	3.01	12	1
1:A:917:THR:HB	1:A:922:PHE:CZ	0.44	2.48	11	3
1:A:960:ARG:HG3	1:A:981:GLN:HB3	0.44	1.89	12	1
1:A:1003:GLU:HG3	1:A:1005:ILE:HG23	0.44	1.89	15	1
1:A:913:LEU:HD23	1:A:914:LYS:N	0.44	2.28	19	1
1:A:934:PRO:O	1:A:1006:LEU:HD22	0.44	2.13	11	1
1:A:993:GLY:O	1:A:1022:ARG:HA	0.44	2.13	13	1
1:A:1006:LEU:HD11	1:A:1009:ASN:C	0.44	2.38	15	1
1:A:975:HIS:O	1:A:977:ILE:HG13	0.44	2.13	2	2
1:A:999:HIS:ND1	1:A:1000:SER:N	0.44	2.66	3	1
1:A:915:THR:HG23	1:A:916:GLN:NE2	0.44	2.27	4	1
1:A:954:PRO:C	1:A:956:ASP:H	0.44	2.21	4	1
1:A:933:ARG:HG2	1:A:934:PRO:HD2	0.44	1.88	5	1
1:A:979:ASP:O	1:A:980:ILE:CG1	0.44	2.66	17	2
1:A:913:LEU:HD21	1:A:915:THR:CG2	0.44	2.43	18	1
1:A:936:TYR:HA	1:A:961:LYS:N	0.44	2.27	18	1
1:A:1006:LEU:HA	1:A:1011:ALA:HA	0.44	1.89	21	1
1:A:1006:LEU:HD22	1:A:1007:SER:H	0.43	1.72	12	1
1:A:928:LEU:O	1:A:942:SER:O	0.43	2.35	3	1
1:A:1012:HIS:CD2	1:A:1012:HIS:N	0.43	2.85	12	1
1:A:955:LYS:HG2	1:A:956:ASP:H	0.43	1.73	16	1
1:A:915:THR:HG23	1:A:916:GLN:N	0.43	2.27	18	1
1:A:912:LYS:HD3	1:A:912:LYS:N	0.43	2.28	3	1
1:A:913:LEU:HD11	1:A:916:GLN:O	0.43	2.13	12	1
1:A:952:SER:O	1:A:954:PRO:HD3	0.43	2.12	10	4
1:A:943:ILE:O	1:A:943:ILE:HG13	0.43	2.14	14	3
1:A:941:PHE:CD1	1:A:957:VAL:HB	0.43	2.48	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1005:ILE:O	1:A:1012:HIS:O	0.43	2.36	12	1
1:A:999:HIS:CD2	1:A:1015:THR:HB	0.43	2.48	15	2
1:A:915:THR:CG2	1:A:917:THR:HG23	0.43	2.43	18	1
1:A:960:ARG:HG3	1:A:981:GLN:OE1	0.43	2.14	19	1
1:A:986:ILE:HG12	1:A:1002:ALA:O	0.43	2.13	3	2
1:A:966:PRO:HG3	1:A:986:ILE:HD12	0.43	1.91	10	1
1:A:924:ILE:HA	1:A:945:CYS:CB	0.43	2.44	11	2
1:A:915:THR:OG1	1:A:929:LYS:HB3	0.43	2.14	22	1
1:A:1016:LYS:HD3	1:A:1017:PRO:O	0.43	2.14	2	1
1:A:969:PRO:HB3	1:A:1019:ILE:HA	0.43	1.90	13	1
1:A:977:ILE:HG13	1:A:985:ARG:O	0.43	2.13	15	1
1:A:980:ILE:HB	1:A:1013:TRP:CZ2	0.43	2.48	17	1
1:A:1004:CYS:HB2	1:A:1013:TRP:CZ3	0.43	2.49	21	1
1:A:908:PHE:CZ	1:A:943:ILE:HD13	0.43	2.49	23	1
1:A:927:SER:HA	1:A:943:ILE:O	0.43	2.14	4	3
1:A:946:LEU:HD11	1:A:952:SER:OG	0.43	2.14	7	1
1:A:937:TYR:CE1	1:A:959:LYS:HB2	0.43	2.49	20	3
1:A:997:ILE:HB	1:A:1019:ILE:H	0.43	1.74	10	1
1:A:991:THR:HG23	1:A:992:THR:N	0.43	2.29	14	1
1:A:1006:LEU:HD12	1:A:1010:THR:O	0.43	2.13	15	1
1:A:905:PRO:HG2	1:A:930:TYR:OH	0.43	2.14	23	1
1:A:966:PRO:HD3	1:A:1013:TRP:CZ2	0.43	2.48	1	1
1:A:941:PHE:CD2	1:A:957:VAL:HG21	0.43	2.48	3	1
1:A:901:HIS:HB2	1:A:921:ASP:HB2	0.43	1.90	13	1
1:A:1006:LEU:O	1:A:1010:THR:O	0.43	2.37	18	1
1:A:986:ILE:HD13	1:A:1013:TRP:CH2	0.43	2.49	21	1
1:A:988:TYR:OH	1:A:1017:PRO:HB3	0.43	2.14	24	1
1:A:905:PRO:HB3	1:A:951:TRP:CD2	0.43	2.48	3	1
1:A:937:TYR:HB3	1:A:961:LYS:CE	0.43	2.44	4	1
1:A:924:ILE:HG22	1:A:925:GLY:N	0.43	2.29	19	6
1:A:991:THR:O	1:A:992:THR:OG1	0.43	2.28	7	1
1:A:1006:LEU:HD13	1:A:1007:SER:CA	0.43	2.44	12	1
1:A:955:LYS:HB3	1:A:956:ASP:H	0.43	1.51	18	1
1:A:939:ARG:NH1	1:A:941:PHE:HB3	0.43	2.29	19	1
1:A:946:LEU:HB2	1:A:950:VAL:HG22	0.42	1.90	20	2
1:A:985:ARG:HE	1:A:1003:GLU:HB3	0.42	1.74	5	1
1:A:903:GLN:C	1:A:903:GLN:NE2	0.42	2.77	10	1
1:A:994:HIS:HB3	1:A:1021:GLN:N	0.42	2.29	14	1
1:A:996:LEU:C	1:A:996:LEU:HD12	0.42	2.39	1	1
1:A:996:LEU:HD21	1:A:999:HIS:O	0.42	2.14	12	1
1:A:916:GLN:NE2	1:A:916:GLN:C	0.42	2.77	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:976:VAL:HB	1:A:980:ILE:HG23	0.42	1.92	17	1
1:A:958:CYS:O	1:A:959:LYS:HE3	0.42	2.15	5	1
1:A:917:THR:HG23	1:A:918:THR:N	0.42	2.29	9	1
1:A:939:ARG:CD	1:A:939:ARG:H	0.42	2.28	19	1
1:A:966:PRO:HG3	1:A:974:VAL:HG21	0.42	1.91	3	1
1:A:903:GLN:NE2	1:A:903:GLN:N	0.42	2.68	13	1
1:A:902:CYS:SG	1:A:922:PHE:O	0.42	2.78	23	1
1:A:935:GLU:HA	1:A:1006:LEU:O	0.42	2.14	24	1
1:A:970:VAL:HG13	1:A:971:ASN:H	0.42	1.74	24	1
1:A:955:LYS:HG2	1:A:956:ASP:OD1	0.42	2.15	3	1
1:A:915:THR:OG1	1:A:929:LYS:HB2	0.42	2.15	4	1
1:A:952:SER:O	1:A:953:SER:C	0.42	2.63	12	1
1:A:992:THR:O	1:A:992:THR:HG23	0.42	2.15	22	1
1:A:903:GLN:NE2	1:A:904:ALA:O	0.42	2.52	10	1
1:A:900:ALA:HA	1:A:949:LEU:HD21	0.42	1.92	11	1
1:A:914:LYS:O	1:A:914:LYS:HG3	0.42	2.15	16	1
1:A:999:HIS:HB2	1:A:1015:THR:HG21	0.42	1.91	22	1
1:A:917:THR:O	1:A:918:THR:OG1	0.42	2.33	4	2
1:A:969:PRO:O	1:A:970:VAL:O	0.42	2.37	11	1
1:A:977:ILE:HD13	1:A:985:ARG:C	0.42	2.40	17	1
1:A:960:ARG:HG2	1:A:981:GLN:NE2	0.42	2.29	21	1
1:A:938:GLY:O	1:A:939:ARG:HG2	0.42	2.15	22	1
1:A:999:HIS:CE1	1:A:1015:THR:HB	0.42	2.50	24	1
1:A:1006:LEU:HD23	1:A:1007:SER:N	0.42	2.29	10	2
1:A:915:THR:CG2	1:A:928:LEU:HD12	0.42	2.45	11	1
1:A:970:VAL:O	1:A:971:ASN:HB2	0.42	2.14	13	2
1:A:1008:GLY:C	1:A:1010:THR:H	0.42	2.23	17	1
1:A:1016:LYS:HD3	1:A:1016:LYS:C	0.42	2.40	24	1
1:A:934:PRO:O	1:A:935:GLU:CB	0.42	2.68	21	3
1:A:982:VAL:HG22	1:A:1004:CYS:SG	0.41	2.55	12	1
1:A:932:CYS:SG	1:A:936:TYR:HB2	0.41	2.55	13	1
1:A:962:SER:HB2	1:A:981:GLN:HG2	0.41	1.93	2	1
1:A:984:SER:O	1:A:1003:GLU:HG3	0.41	2.15	20	2
1:A:1006:LEU:HD13	1:A:1007:SER:O	0.41	2.15	24	1
1:A:937:TYR:HB3	1:A:961:LYS:HE3	0.41	1.92	4	1
1:A:941:PHE:CD1	1:A:957:VAL:HG21	0.41	2.51	19	1
1:A:908:PHE:CD1	1:A:908:PHE:N	0.41	2.89	2	1
1:A:1021:GLN:C	1:A:1023:ILE:N	0.41	2.78	6	1
1:A:977:ILE:HG12	1:A:985:ARG:O	0.41	2.14	9	1
1:A:936:TYR:CD1	1:A:936:TYR:N	0.41	2.88	24	2
1:A:902:CYS:O	1:A:921:ASP:HA	0.41	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:970:VAL:O	1:A:1020:CYS:HB3	0.41	2.14	7	1
1:A:916:GLN:HG2	1:A:916:GLN:O	0.41	2.16	9	1
1:A:986:ILE:HG12	1:A:1013:TRP:CZ3	0.41	2.50	18	1
1:A:908:PHE:CE2	1:A:943:ILE:HD13	0.41	2.51	23	1
1:A:955:LYS:HB2	1:A:955:LYS:HZ2	0.41	1.75	1	1
1:A:960:ARG:HB3	1:A:981:GLN:HB3	0.41	1.92	16	1
1:A:988:TYR:CD1	1:A:988:TYR:N	0.41	2.89	19	1
1:A:997:ILE:HD13	1:A:1021:GLN:HG2	0.41	1.90	1	1
1:A:981:GLN:C	1:A:983:GLY:N	0.41	2.79	9	2
1:A:930:TYR:O	1:A:940:PRO:HA	0.41	2.16	10	1
1:A:916:GLN:O	1:A:917:THR:CG2	0.41	2.69	12	1
1:A:935:GLU:C	1:A:961:LYS:HG2	0.41	2.41	15	1
1:A:974:VAL:HG13	1:A:976:VAL:HG23	0.41	1.92	18	1
1:A:995:ARG:HD2	1:A:996:LEU:N	0.41	2.30	24	1
1:A:909:LEU:HD12	1:A:909:LEU:N	0.41	2.30	1	1
1:A:976:VAL:HG12	1:A:986:ILE:HG22	0.41	1.92	1	1
1:A:934:PRO:O	1:A:1006:LEU:HD12	0.41	2.16	2	1
1:A:982:VAL:HG11	1:A:1006:LEU:HG	0.41	1.91	2	1
1:A:928:LEU:HB2	1:A:930:TYR:HE1	0.41	1.76	3	1
1:A:928:LEU:O	1:A:942:SER:HB3	0.41	2.15	5	1
1:A:935:GLU:N	1:A:1006:LEU:HD22	0.41	2.30	14	1
1:A:976:VAL:C	1:A:977:ILE:HG12	0.41	2.40	15	1
1:A:908:PHE:O	1:A:910:PHE:N	0.41	2.54	16	1
1:A:963:CYS:HB2	1:A:1013:TRP:CE2	0.41	2.51	18	1
1:A:964:LYS:HD3	1:A:965:THR:O	0.41	2.16	18	1
1:A:974:VAL:HG22	1:A:975:HIS:H	0.41	1.76	3	1
1:A:995:ARG:HE	1:A:1023:ILE:HG12	0.40	1.76	6	1
1:A:961:LYS:CG	1:A:962:SER:N	0.40	2.82	12	1
1:A:913:LEU:HG	1:A:930:TYR:CE2	0.40	2.51	13	1
1:A:935:GLU:C	1:A:961:LYS:HB2	0.40	2.41	14	1
1:A:962:SER:OG	1:A:981:GLN:HG2	0.40	2.16	20	1
1:A:937:TYR:HB3	1:A:961:LYS:HD3	0.40	1.91	2	1
1:A:906:ASP:C	1:A:907:HIS:ND1	0.40	2.79	12	1
1:A:988:TYR:CD2	1:A:1018:PRO:HG2	0.40	2.51	19	1
1:A:937:TYR:CE2	1:A:961:LYS:HA	0.40	2.52	20	1
1:A:1016:LYS:HD3	1:A:1017:PRO:N	0.40	2.31	22	1
1:A:1009:ASN:N	1:A:1009:ASN:ND2	0.40	2.69	2	1
1:A:915:THR:O	1:A:916:GLN:C	0.40	2.65	12	1
1:A:1017:PRO:HA	1:A:1018:PRO:HD2	0.40	1.84	19	1
1:A:916:GLN:CD	1:A:917:THR:H	0.40	2.25	23	1
1:A:992:THR:HG23	1:A:993:GLY:N	0.40	2.31	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:905:PRO:HB3	1:A:951:TRP:CE2	0.40	2.51	11	1
1:A:910:PHE:CD1	1:A:958:CYS:HB2	0.40	2.51	12	1
1:A:914:LYS:HB2	1:A:931:GLU:HG3	0.40	1.94	13	1
1:A:901:HIS:N	1:A:949:LEU:HD11	0.40	2.31	17	1
1:A:900:ALA:HB3	1:A:924:ILE:HD11	0.40	1.92	19	1
1:A:1006:LEU:CD1	1:A:1007:SER:N	0.40	2.84	24	1
1:A:972:GLY:O	1:A:973:MET:HB2	0.40	2.17	3	1
1:A:959:LYS:HD2	1:A:959:LYS:N	0.40	2.28	8	1
1:A:961:LYS:HE2	1:A:1006:LEU:HD13	0.40	1.92	9	1
1:A:980:ILE:HG22	1:A:986:ILE:HG21	0.40	1.92	12	1
1:A:987:THR:HG22	1:A:1001:SER:OG	0.40	2.17	15	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	124/128 (97%)	91±4 (73±3%)	23±4 (18±3%)	11±3 (9±2%)	1	12
All	All	2976/3072 (97%)	2173 (73%)	541 (18%)	262 (9%)	1	12

All 52 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	982	VAL	17
1	A	1000	SER	16
1	A	999	HIS	15
1	A	1018	PRO	15
1	A	947	ASP	14
1	A	957	VAL	14
1	A	980	ILE	11
1	A	964	LYS	11
1	A	1008	GLY	10
1	A	938	GLY	9
1	A	939	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	935	GLU	8
1	A	900	ALA	8
1	A	973	MET	7
1	A	992	THR	7
1	A	906	ASP	5
1	A	915	THR	5
1	A	901	HIS	5
1	A	955	LYS	4
1	A	983	GLY	4
1	A	956	ASP	4
1	A	1009	ASN	4
1	A	953	SER	4
1	A	916	GLN	3
1	A	943	ILE	3
1	A	907	HIS	3
1	A	990	CYS	3
1	A	1005	ILE	3
1	A	979	ASP	3
1	A	968	ASP	3
1	A	1019	ILE	3
1	A	905	PRO	3
1	A	977	ILE	2
1	A	954	PRO	2
1	A	998	GLY	2
1	A	1022	ARG	2
1	A	932	CYS	2
1	A	969	PRO	2
1	A	917	THR	2
1	A	952	SER	2
1	A	1006	LEU	2
1	A	940	PRO	1
1	A	918	THR	1
1	A	961	LYS	1
1	A	1023	ILE	1
1	A	919	ALA	1
1	A	970	VAL	1
1	A	984	SER	1
1	A	1007	SER	1
1	A	909	LEU	1
1	A	960	ARG	1
1	A	991	THR	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	112/114 (98%)	108±2 (96±2%)	4±2 (4±2%)	32 82
All	All	2688/2736 (98%)	2591 (96%)	97 (4%)	32 82

All 31 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	1019	ILE	11
1	A	910	PHE	10
1	A	1016	LYS	7
1	A	916	GLN	7
1	A	944	THR	6
1	A	955	LYS	5
1	A	975	HIS	5
1	A	1021	GLN	5
1	A	903	GLN	4
1	A	960	ARG	3
1	A	939	ARG	3
1	A	909	LEU	3
1	A	914	LYS	3
1	A	929	LYS	2
1	A	950	VAL	2
1	A	912	LYS	2
1	A	964	LYS	2
1	A	961	LYS	2
1	A	937	TYR	2
1	A	957	VAL	2
1	A	1005	ILE	1
1	A	906	ASP	1
1	A	913	LEU	1
1	A	1012	HIS	1
1	A	976	VAL	1
1	A	996	LEU	1
1	A	982	VAL	1
1	A	1010	THR	1
1	A	948	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	973	MET	1
1	A	970	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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