Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 07:37 pm BST

PDB ID	:	1GKN
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

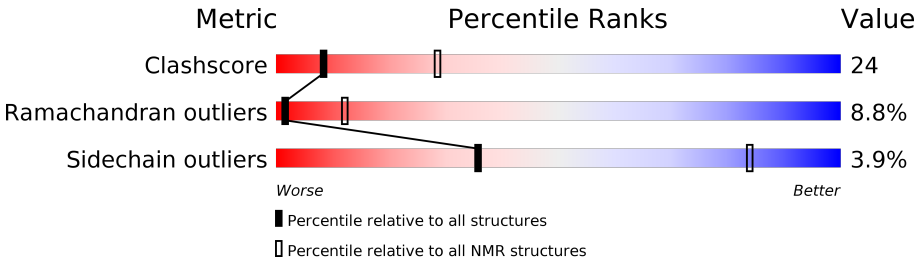
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	128	42% 55% .

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)	0.98	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 3 clusters and 2 single-model clusters were found.

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

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

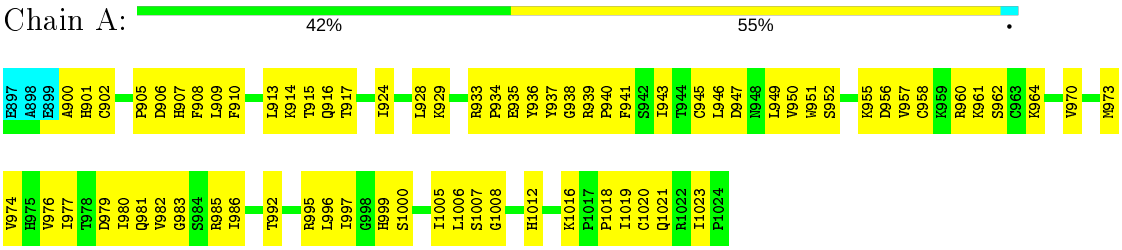
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

Chain A:



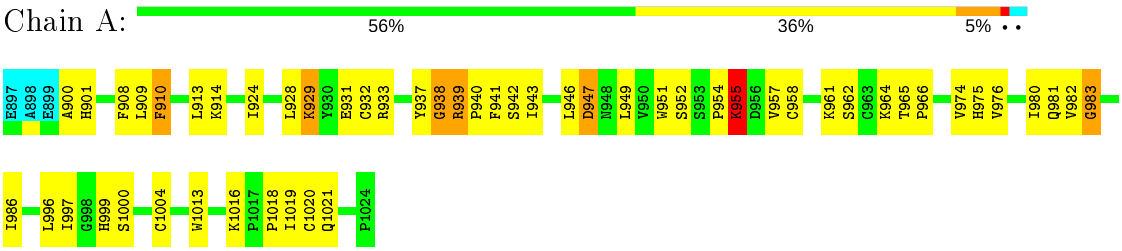
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

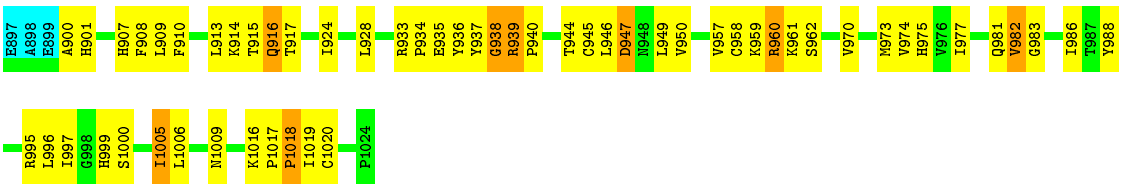
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

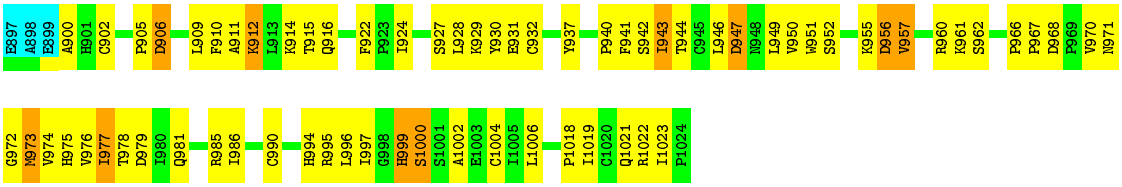
Chain A:



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

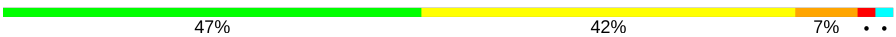
Chain A:

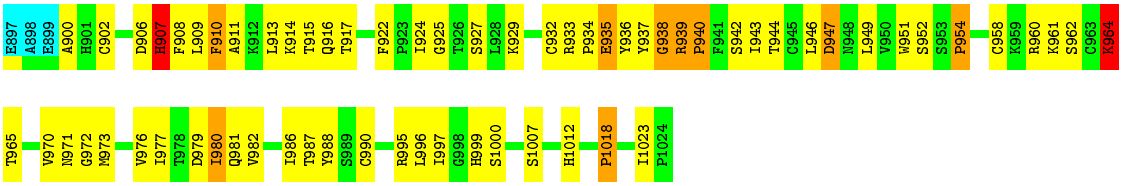


4.2.4 Score per residue for model 4

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A:

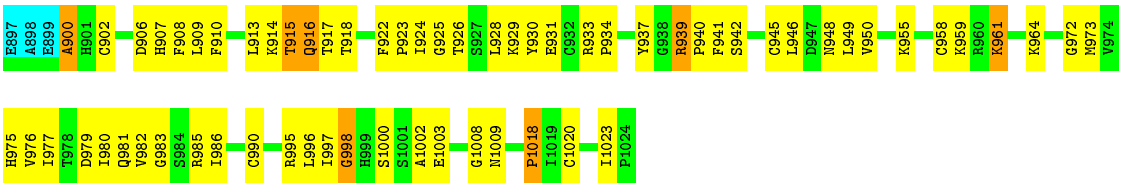




4.2.5 Score per residue for model 5

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

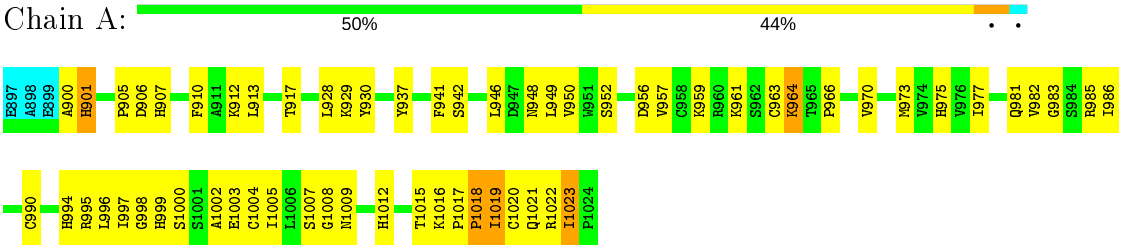
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

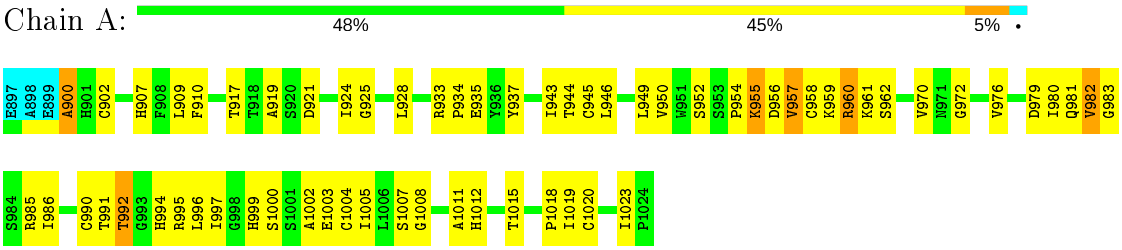
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

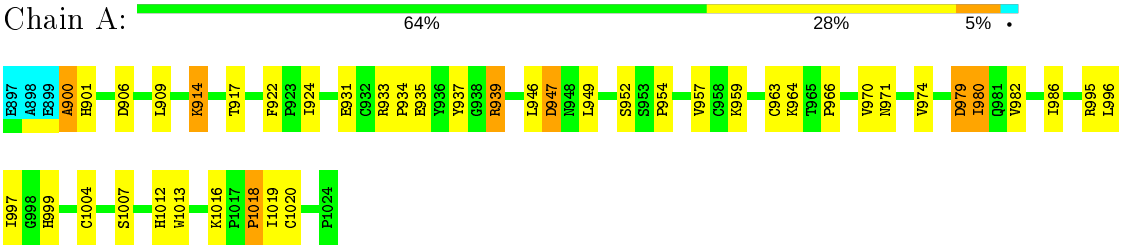
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

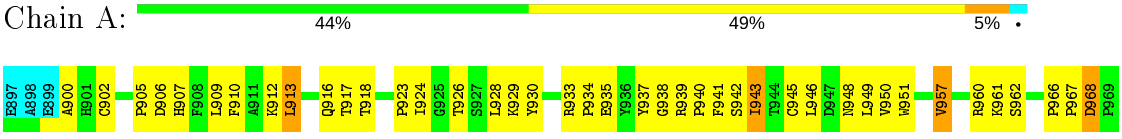
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

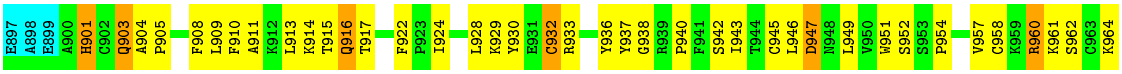
Chain A:

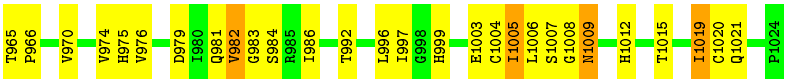


4.2.10 Score per residue for model 10

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A:

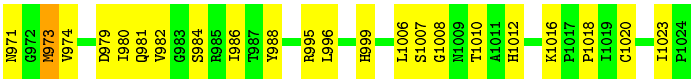




4.2.11 Score per residue for model 11

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

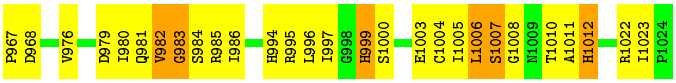
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

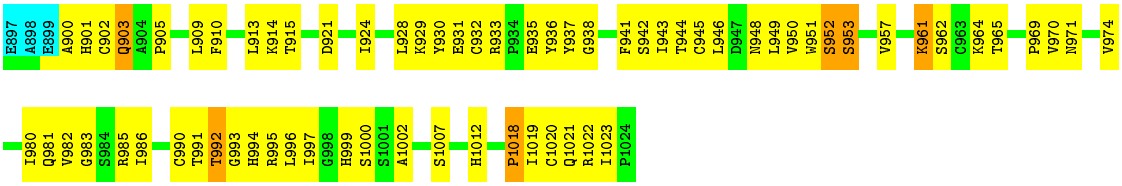
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

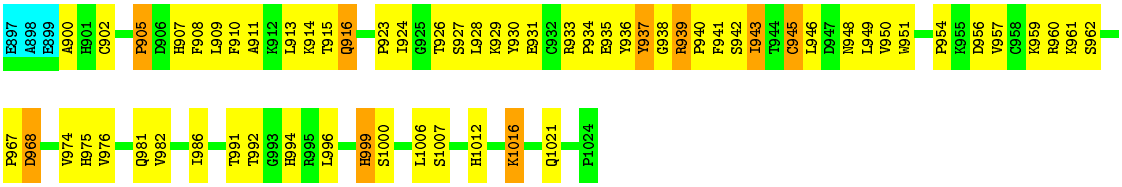
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

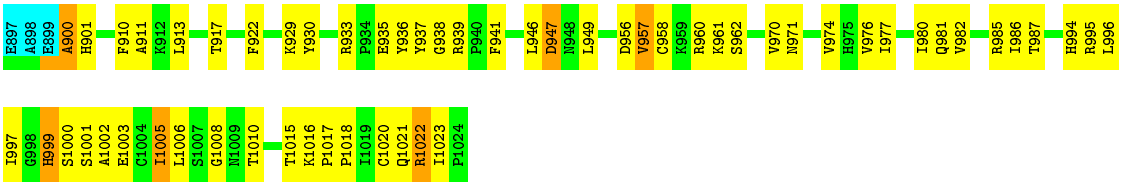
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

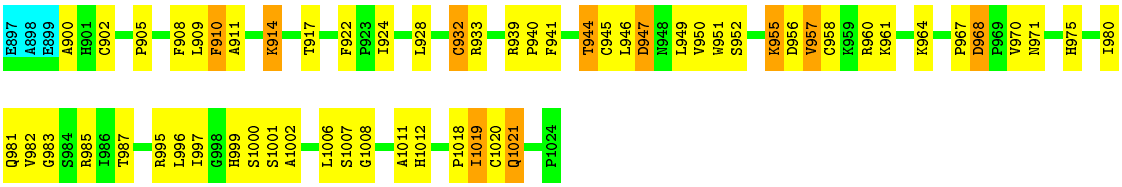
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: COMPLEMENT RECEPTOR TYPE 1

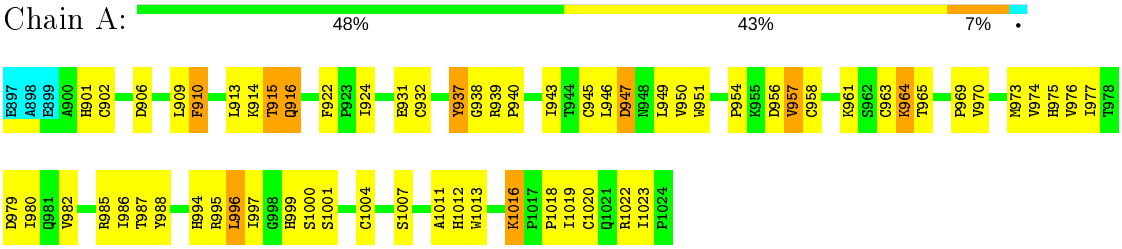
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

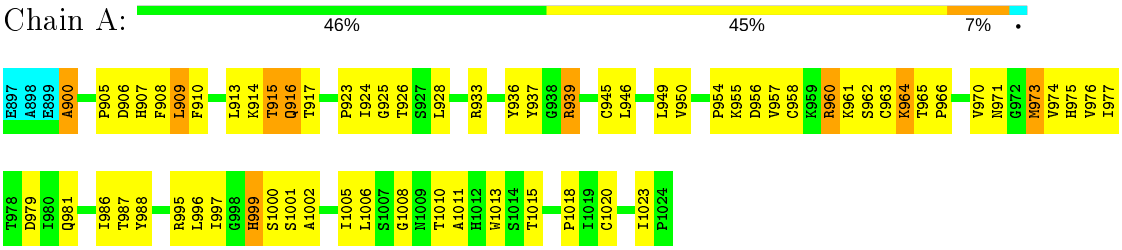
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

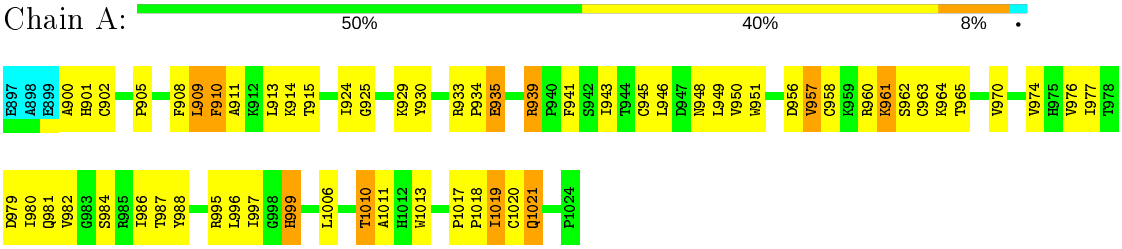
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

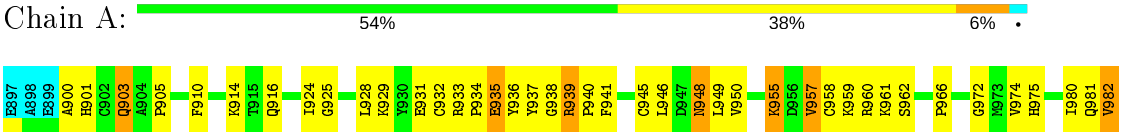
Chain A:

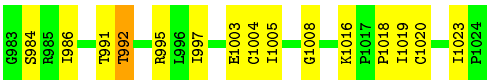


4.2.20 Score per residue for model 20

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A:

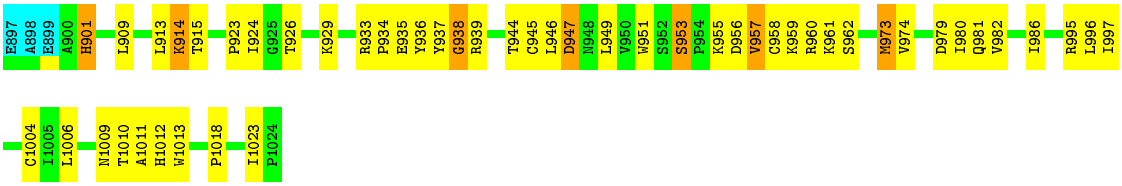




4.2.21 Score per residue for model 21

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

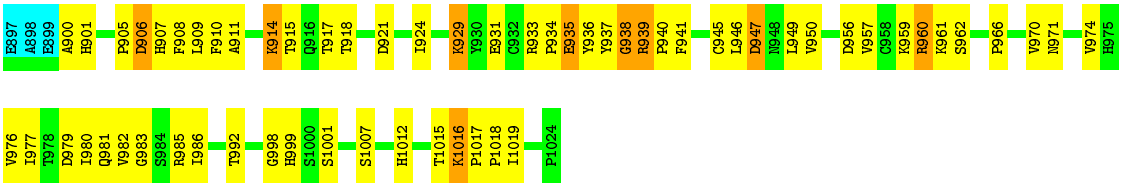
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

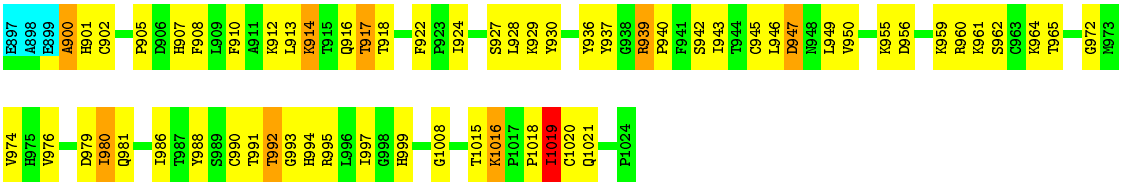
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

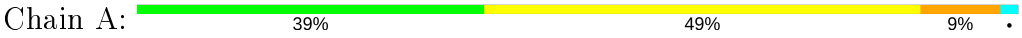
Chain A:

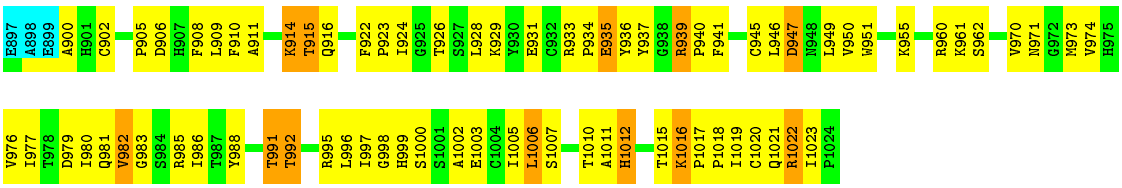


4.2.24 Score per residue for model 24

• Molecule 1: COMPLEMENT RECEPTOR TYPE 1

Chain A:




E897
A898
E899
A900
H901
C902
P905
D906
H907
F908
L909
F910
A911
K914
T915
Q916
F922
P923
I924
G925
T926
S927
L928
K929
Y930
E931
C932
R933
P934
E935
Y936
Y937
G938
R939
P940
F941
C945
L946
D947
N948
L949
V950
W951
K955
R960
K961
S962
V970
N971
G972
H973
V974
H975
V976
I977
T978
D979
I980
Q981
V982
G983
S984
R985
I986
T987
Y988
T991
T992
R995
L996
I997
G998
H999
S1000
S1001
A1002
E1003
C1004
I1005
L1006
S1007
T1010
A1011
H1012
T1015
K1016
P1017
P1018
I1019
C1020
Q1021
R1022
I1023
P1024

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 VERSION:	structure solution	1.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	46±10
All	All	23304	22968	22824	1114

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 24.

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:HE2	1:A:959:LYS:HA	0.70	1.63	12	2
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:HE2	1:A:914:LYS:HA	0.67	1.67	22	1
1:A:946:LEU:N	1:A:946:LEU:HD22	0.67	2.03	14	7
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	3
1:A:909:LEU:N	1:A:909:LEU:HD22	0.64	2.06	18	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:924:ILE:HD13	1:A:945:CYS:SG	0.63	2.34	2	1
1:A:990:CYS:SG	1:A:994:HIS:HB2	0.63	2.34	7	1
1:A:946:LEU:HD22	1:A:946:LEU:N	0.63	2.09	13	4
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:959:LYS:HA	1:A:959:LYS:HE2	0.62	1.71	5	1
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:961:LYS:HZ2	1:A:961:LYS:HB2	0.62	1.55	10	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:HA	1:A:964:LYS:HE3	0.61	1.71	4	1
1:A:929:LYS:HA	1:A:942:SER:HA	0.61	1.72	9	2
1:A:962:SER:HB3	1:A:981:GLN:HE21	0.60	1.56	11	4
1:A:957:VAL:HG23	1:A:958:CYS:H	0.60	1.56	15	6
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: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:NZ	1:A:961:LYS:HB2	0.59	2.13	10	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	1
1:A:999:HIS:ND1	1:A:1015:THR:HB	0.58	2.13	24	1
1:A:908:PHE:O	1:A:909:LEU:HD13	0.58	1.97	18	1
1:A:916:GLN:H	1:A:916:GLN:NE2	0.58	1.96	14	2
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:913:LEU:HD11	1:A:915:THR:HG22	0.57	1.75	18	1
1:A:961:LYS:CG	1:A:982:VAL:HG22	0.57	2.30	19	1
1:A:955:LYS:NZ	1:A:955:LYS:HB2	0.57	2.15	7	2
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: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:1006:LEU:HD12	1:A:1010:THR:C	0.56	2.21	18	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:HD3	1:A:1016:LYS:O	0.55	2.01	24	1
1:A:929:LYS:HB2	1:A:929:LYS:NZ	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:1016:LYS:HB3	1:A:1016:LYS:NZ	0.55	2.17	11	1
1:A:1007:SER:HA	1:A:1010:THR:O	0.55	2.01	12	2
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:HB3	1:A:955:LYS:NZ	0.54	2.18	24	1
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: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:CD1	1:A:909:LEU:N	0.54	2.71	19	2
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:HD12	1:A:909:LEU:N	0.53	2.18	3	3
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: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:955:LYS:HB2	1:A:955:LYS:NZ	0.53	2.19	20	1
1:A:911:ALA:HA	1:A:932:CYS:HA	0.53	1.79	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:962:SER:HB3	1:A:981:GLN:OE1	0.53	2.04	9	1
1:A:914:LYS:NZ	1:A:914:LYS:HB3	0.53	2.18	20	2
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:NZ	1:A:912:LYS:HB2	0.52	2.20	6	1
1:A:913:LEU:HD21	1:A:917:THR:HG23	0.52	1.82	11	1
1:A:979:ASP:O	1:A:980:ILE:HG12	0.52	2.05	17	2
1:A:901:HIS:C	1:A:949:LEU:HD22	0.52	2.26	20	3
1:A:976:VAL:O	1:A:977:ILE:HB	0.52	2.04	3	1
1:A:902:CYS:O	1:A:922:PHE:HB2	0.52	2.05	11	5
1:A:948:ASN:H	1:A:948:ASN:ND2	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:1006:LEU:C	1:A:1006:LEU:HD13	0.51	2.24	12	2
1:A:937:TYR:HB3	1:A:961:LYS:NZ	0.51	2.20	21	2
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: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: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
1:A:986:ILE:HG13	1:A:986:ILE:O	0.51	2.06	18	2
1:A:991:THR:O	1:A:992:THR:C	0.51	2.49	24	2
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:905:PRO:HG3	1:A:951:TRP:CE2	0.51	2.41	24	2
1:A:963:CYS:SG	1:A:1013:TRP:CE2	0.51	3.04	8	2
1:A:996:LEU:C	1:A:997:ILE:HD12	0.51	2.25	1	1
1:A:991:THR:O	1:A:992:THR:OG1	0.51	2.28	7	1
1:A:915:THR:HG22	1:A:916:GLN:NE2	0.51	2.20	24	1
1:A:937:TYR:HB3	1:A:961:LYS:HZ2	0.51	1.66	12	1
1:A:905:PRO:HG2	1:A:928:LEU:HD23	0.51	1.83	16	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:908:PHE:O	1:A:909:LEU:HB2	0.50	2.06	1	4
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:914:LYS:O	1:A:915:THR:C	0.50	2.50	5	1
1:A:935:GLU:HB3	1:A:982:VAL:HG11	0.50	1.82	12	1
1:A:909:LEU:HD12	1:A:909:LEU:C	0.50	2.26	17	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:946:LEU:N	1:A:946:LEU:CD2	0.50	2.75	14	5
1:A:986:ILE:O	1:A:986:ILE:HG13	0.50	2.07	21	2
1:A:961:LYS:HG2	1:A:1007:SER:CB	0.50	2.35	12	1
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:HD3	1:A:955:LYS:N	0.49	2.22	12	1
1:A:961:LYS:HB2	1:A:961:LYS:NZ	0.49	2.22	13	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:987:THR:HA	1:A:1001:SER:HA	0.49	1.83	18	1
1:A:939:ARG:HD2	1:A:939:ARG:C	0.49	2.27	24	1
1:A:913:LEU:HD13	1:A:930:TYR:CE1	0.49	2.43	15	1
1:A:908:PHE:C	1:A:909:LEU:HD13	0.49	2.28	18	1
1:A:916:GLN:O	1:A:917:THR:HG22	0.49	2.07	12	1
1:A:962:SER:HB3	1:A:981:GLN:HG3	0.49	1.84	13	1
1:A:903:GLN:NE2	1:A:903:GLN:H	0.49	2.05	20	2
1:A:1005:ILE:HD13	1:A:1005:ILE:H	0.49	1.68	2	1
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:964:LYS:HB3	1:A:964:LYS:NZ	0.49	2.22	6	1
1:A:916:GLN:H	1:A:916:GLN:CD	0.49	2.11	9	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:1019:ILE:HD12	1:A:1019:ILE:H	0.49	1.67	19	1
1:A:1016:LYS:O	1:A:1016:LYS:HD2	0.49	2.08	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:916:GLN:O	1:A:917:THR:O	0.49	2.31	23	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: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:909:LEU:HD22	1:A:909:LEU:C	0.48	2.28	19	1
1:A:946:LEU:HD11	1:A:952:SER:HA	0.48	1.85	16	1
1:A:913:LEU:HD13	1:A:913:LEU:C	0.48	2.29	18	3
1:A:914:LYS:HE2	1:A:929:LYS:HD2	0.48	1.84	21	1
1:A:960:ARG:HD2	1:A:982:VAL:HB	0.48	1.85	24	1
1:A:996:LEU:HD21	1:A:1018:PRO:HB3	0.48	1.85	24	2
1:A:928:LEU:HD23	1:A:930:TYR:CE1	0.48	2.44	5	1
1:A:935:GLU:C	1:A:961:LYS:HB3	0.48	2.29	19	1
1:A:961:LYS:CD	1:A:1007:SER:HB2	0.48	2.39	24	1
1:A:994:HIS:HA	1:A:1021:GLN:O	0.48	2.09	6	1
1:A:967:PRO:O	1:A:968:ASP:C	0.48	2.52	12	4
1:A:909:LEU:N	1:A:909:LEU:CD1	0.48	2.77	14	2
1:A:948:ASN:ND2	1:A:948:ASN:N	0.48	2.61	20	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:946:LEU:HB2	1:A:950:VAL:HG23	0.47	1.85	24	4
1:A:951:TRP:O	1:A:954:PRO:HD3	0.47	2.09	17	1
1:A:913:LEU:C	1:A:913:LEU:HD13	0.47	2.29	17	6
1:A:936:TYR:C	1:A:961:LYS:HE2	0.47	2.30	12	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:935:GLU:C	1:A:961:LYS:HD3	0.47	2.29	21	1
1:A:910:PHE:O	1:A:932:CYS:HA	0.47	2.10	17	4
1:A:1016:LYS:HD2	1:A:1016:LYS:O	0.47	2.09	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:HD12	1:A:996:LEU:O	0.47	2.09	1	1
1:A:988:TYR:CD2	1:A:1018:PRO:HD2	0.47	2.45	2	3
1:A:937:TYR:O	1:A:958:CYS:HA	0.47	2.10	4	1
1:A:933:ARG:HB3	1:A:934:PRO:HD2	0.47	1.86	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1021:GLN:C	1:A:1023:ILE:H	0.47	2.12	6	1
1:A:900:ALA:HA	1:A:949:LEU:HD11	0.47	1.85	6	2
1:A:991:THR:O	1:A:993:GLY:N	0.47	2.48	9	1
1:A:905:PRO:HG3	1:A:951:TRP:CZ2	0.47	2.44	10	2
1:A:901:HIS:C	1:A:949:LEU:HD12	0.47	2.30	17	2
1:A:961:LYS:HG3	1:A:982:VAL:HG22	0.47	1.86	19	1
1:A:924:ILE:HA	1:A:945:CYS:HB3	0.47	1.85	21	2
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:981:GLN:C	1:A:983:GLY:H	0.47	2.14	9	3
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:996:LEU:HD13	1:A:996:LEU:C	0.47	2.30	19	2
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:966:PRO:HG3	1:A:986:ILE:CD1	0.46	2.41	10	6
1:A:985:ARG:HG3	1:A:1002:ALA:C	0.46	2.31	15	3
1:A:957:VAL:O	1:A:957:VAL:HG23	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:H	1:A:948:ASN:HD22	0.46	1.52	20	1
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:996:LEU:HD23	1:A:996:LEU:C	0.46	2.31	2	6
1:A:925:GLY:O	1:A:944:THR:HG23	0.46	2.10	4	1
1:A:909:LEU:CD2	1:A:909:LEU:N	0.46	2.78	11	3
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:908:PHE:CZ	1:A:954:PRO:HG2	0.45	2.46	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:939:ARG:HD2	1:A:939:ARG:N	0.45	2.26	5	1
1:A:915:THR:HG22	1:A:916:GLN:N	0.45	2.27	17	2
1:A:935:GLU:HG3	1:A:936:TYR:CE1	0.45	2.45	15	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:914:LYS:C	1:A:914:LYS:HD2	0.45	2.31	21	4
1:A:906:ASP:OD1	1:A:907:HIS:N	0.45	2.50	6	4
1:A:985:ARG:HG2	1:A:986:ILE:N	0.45	2.26	17	1
1:A:951:TRP:C	1:A:953:SER:N	0.45	2.70	21	1
1:A:997:ILE:HD11	1:A:1021:GLN:CG	0.45	2.41	6	1
1:A:939:ARG:C	1:A:939:ARG:HD2	0.45	2.31	23	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:939:ARG:N	1:A:939:ARG:HD2	0.45	2.26	18	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:996:LEU:C	1:A:996:LEU:HD23	0.45	2.32	8	6
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:918:THR:O	1:A:918:THR:HG22	0.45	2.12	23	1
1:A:905:PRO:O	1:A:906:ASP:C	0.45	2.56	22	5
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:980:ILE:HG22	1:A:986:ILE:CG2	0.45	2.42	17	1
1:A:946:LEU:CD2	1:A:946:LEU:N	0.44	2.79	18	2
1:A:1005:ILE:O	1:A:1011:ALA:HA	0.44	2.11	18	1
1:A:985:ARG:HG3	1:A:1002:ALA:O	0.44	2.12	16	1
1:A:917:THR:CG2	1:A:928:LEU:HD11	0.44	2.42	2	1
1:A:905:PRO:HB3	1:A:943:ILE:HD11	0.44	1.89	12	1
1:A:903:GLN:H	1:A:903:GLN:CD	0.44	2.15	13	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:979:ASP:HB3	1:A:981:GLN:HG2	0.44	1.88	19	1
1:A:916:GLN:CD	1:A:917:THR:N	0.44	2.70	23	1
1:A:973:MET:SD	1:A:973:MET:N	0.44	2.91	21	2
1:A:996:LEU:HA	1:A:1019:ILE:O	0.44	2.13	1	1
1:A:909:LEU:N	1:A:909:LEU:HD12	0.44	2.28	21	3
1:A:1016:LYS:HD2	1:A:1016:LYS:C	0.44	2.33	8	2
1:A:906:ASP:CG	1:A:907:HIS:H	0.44	2.16	9	2
1:A:913:LEU:CD2	1:A:928:LEU:HB3	0.44	2.43	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:951:TRP:O	1:A:952:SER:C	0.44	2.56	4	2
1:A:906:ASP:CG	1:A:907:HIS:N	0.44	2.71	5	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: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: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:N	1:A:1012:HIS:CD2	0.43	2.85	12	1
1:A:915:THR:HG23	1:A:916:GLN:N	0.43	2.27	18	1
1:A:955:LYS:HG2	1:A:956:ASP:H	0.43	1.73	16	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
1:A:909:LEU:N	1:A:909:LEU:CD2	0.43	2.81	12	3
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:1021:GLN:O	1:A:1022:ARG:C	0.43	2.56	24	1
1:A:986:ILE:HG12	1:A:1002:ALA:O	0.43	2.13	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:997:ILE:HB	1:A:1019:ILE:H	0.43	1.74	10	1
1:A:937:TYR:CE1	1:A:959:LYS:HB2	0.43	2.49	20	3
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:1006:LEU:HD23	1:A:1006:LEU:C	0.43	2.34	10	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:906:ASP:O	1:A:907:HIS:C	0.43	2.57	4	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:1006:LEU:HD13	1:A:1007:SER:CA	0.43	2.44	12	1
1:A:961:LYS:HZ1	1:A:1011:ALA:H	0.43	1.55	17	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:979:ASP:CG	1:A:980:ILE:H	0.43	2.18	8	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:994:HIS:HB3	1:A:1021:GLN:N	0.42	2.29	14	1
1:A:996:LEU:HD21	1:A:999:HIS:O	0.42	2.14	12	1
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:H	1:A:939:ARG:CD	0.42	2.28	19	1
1:A:966:PRO:HG3	1:A:974:VAL:HG21	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:903:GLN:N	1:A:903:GLN:NE2	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:901:HIS:C	1:A:949:LEU:HG	0.42	2.34	8	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: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:951:TRP:C	1:A:953:SER:H	0.42	2.18	21	2
1:A:999:HIS:HB2	1:A:1015:THR:HG21	0.42	1.91	22	1
1:A:914:LYS:HG3	1:A:914:LYS:O	0.42	2.15	16	1
1:A:977:ILE:HG22	1:A:977:ILE:O	0.42	2.15	5	1
1:A:969:PRO:O	1:A:970:VAL:O	0.42	2.37	11	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:955:LYS:C	1:A:955:LYS:HD3	0.42	2.34	23	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: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:973:MET:N	1:A:973:MET:SD	0.41	2.93	18	1
1:A:962:SER:HB2	1:A:981:GLN:HG2	0.41	1.93	2	1
1:A:911:ALA:C	1:A:912:LYS:HD3	0.41	2.35	3	1
1:A:984:SER:O	1:A:1003:GLU:HG3	0.41	2.15	20	2
1:A:934:PRO:C	1:A:936:TYR:H	0.41	2.18	11	1
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:1016:LYS:HD3	1:A:1016:LYS:C	0.41	2.36	22	1
1:A:908:PHE:N	1:A:908:PHE:CD1	0.41	2.89	2	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	1
1:A:902:CYS:O	1:A:921:ASP:HA	0.41	2.16	7	1
1:A:970:VAL:O	1:A:1020:CYS:HB3	0.41	2.14	7	1
1:A:916:GLN:O	1:A:916:GLN:HG2	0.41	2.16	9	1
1:A:986:ILE:HG12	1:A:1013:TRP:CZ3	0.41	2.50	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:908:PHE:CE2	1:A:943:ILE:HD13	0.41	2.51	23	1
1:A:1016:LYS:C	1:A:1016:LYS:HD2	0.41	2.35	9	1
1:A:988:TYR:CD1	1:A:988:TYR:N	0.41	2.89	19	1
1:A:960:ARG:HB3	1:A:981:GLN:HB3	0.41	1.92	16	1
1:A:997:ILE:HD13	1:A:1021:GLN:HG2	0.41	1.90	1	1
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: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:936:TYR:N	1:A:936:TYR:CD1	0.41	2.87	20	1
1:A:976:VAL:HG12	1:A:986:ILE:HG22	0.41	1.92	1	1
1:A:982:VAL:HG11	1:A:1006:LEU:HG	0.41	1.91	2	1
1:A:934:PRO:O	1:A:1006:LEU:HD12	0.41	2.16	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:C	1:A:961:LYS:HG3	0.41	2.36	9	1
1:A:935:GLU:N	1:A:1006:LEU:HD22	0.41	2.30	14	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:917:THR:O	1:A:918:THR:OG1	0.41	2.33	22	1
1:A:908:PHE:O	1:A:910:PHE:N	0.41	2.54	16	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:910:PHE:C	1:A:933:ARG:HG3	0.40	2.36	20	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: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:ND2	1:A:1009:ASN:N	0.40	2.69	2	1
1:A:1017:PRO:HA	1:A:1018:PRO:HD2	0.40	1.84	19	1
1:A:992:THR:HG23	1:A:993:GLY:N	0.40	2.31	23	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:959:LYS:HD2	1:A:959:LYS:N	0.40	2.28	8	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	957	VAL	14
1	A	947	ASP	14
1	A	964	LYS	11
1	A	980	ILE	11
1	A	1008	GLY	10
1	A	939	ARG	9
1	A	938	GLY	9
1	A	935	GLU	8
1	A	900	ALA	8
1	A	992	THR	7
1	A	973	MET	7
1	A	915	THR	5
1	A	906	ASP	5
1	A	901	HIS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	955	LYS	4
1	A	956	ASP	4
1	A	983	GLY	4
1	A	953	SER	4
1	A	1009	ASN	4
1	A	905	PRO	3
1	A	1005	ILE	3
1	A	979	ASP	3
1	A	907	HIS	3
1	A	968	ASP	3
1	A	916	GLN	3
1	A	1019	ILE	3
1	A	943	ILE	3
1	A	990	CYS	3
1	A	952	SER	2
1	A	932	CYS	2
1	A	1006	LEU	2
1	A	954	PRO	2
1	A	998	GLY	2
1	A	917	THR	2
1	A	977	ILE	2
1	A	969	PRO	2
1	A	1022	ARG	2
1	A	909	LEU	1
1	A	991	THR	1
1	A	940	PRO	1
1	A	960	ARG	1
1	A	1023	ILE	1
1	A	918	THR	1
1	A	961	LYS	1
1	A	970	VAL	1
1	A	984	SER	1
1	A	1007	SER	1
1	A	919	ALA	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	112/114 (98%)	108±2 (96±1%)	4±2 (4±1%)	36 84
All	All	2688/2736 (98%)	2583 (96%)	105 (4%)	36 84

All 32 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	910	PHE	19
1	A	1016	LYS	6
1	A	939	ARG	6
1	A	914	LYS	6
1	A	916	GLN	6
1	A	975	HIS	6
1	A	1021	GLN	5
1	A	960	ARG	5
1	A	1019	ILE	4
1	A	909	LEU	3
1	A	903	GLN	3
1	A	955	LYS	3
1	A	907	HIS	3
1	A	1012	HIS	3
1	A	973	MET	3
1	A	929	LYS	2
1	A	912	LYS	2
1	A	957	VAL	2
1	A	944	THR	2
1	A	961	LYS	2
1	A	950	VAL	2
1	A	937	TYR	2
1	A	906	ASP	1
1	A	1005	ILE	1
1	A	996	LEU	1
1	A	948	ASN	1
1	A	945	CYS	1
1	A	913	LEU	1
1	A	964	LYS	1
1	A	1009	ASN	1
1	A	1022	ARG	1
1	A	1010	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided