



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 04:48 PM UTC

PDB ID : 2FIN / pdb_00002fin
Title : Solution Structure of the complex between poxvirus-encoded CC chemokine inhibitor vCCI and human MIP-1beta, ensemble structure
Authors : Zhang, L.
Deposited on : 2005-12-29

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

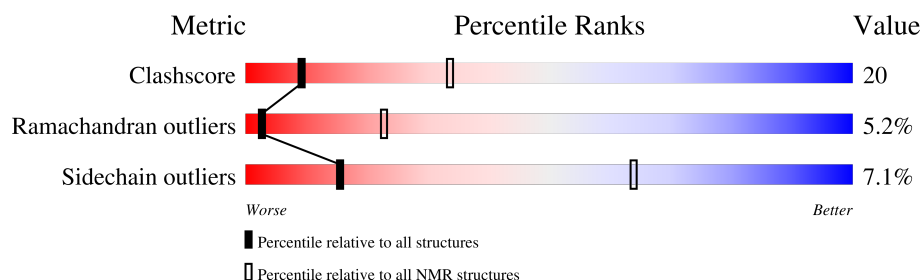
1 Overall quality at a glance

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	242	
2	B	69	

2 Ensemble composition and analysis

This entry contains 15 models. Model 15 is the overall representative, medoid model (most similar to other models).

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:8-A:54, A:77-A:242, B:10-B:69 (273)	0.54	15

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4601 atoms, of which 2247 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called rabbitpox encoded CC chemokine inhibitor.

Mol	Chain	Residues	Atoms						Trace
1	A	242	Total	C	H	N	O	S	0
			3575	1104	1755	298	405	13	

- Molecule 2 is a protein called Small inducible cytokine A4.

Mol	Chain	Residues	Atoms						Trace
2	B	69	Total	C	H	N	O	S	0
			1026	337	492	83	109	5	

There are 3 discrepancies between the modelled and reference sequences:

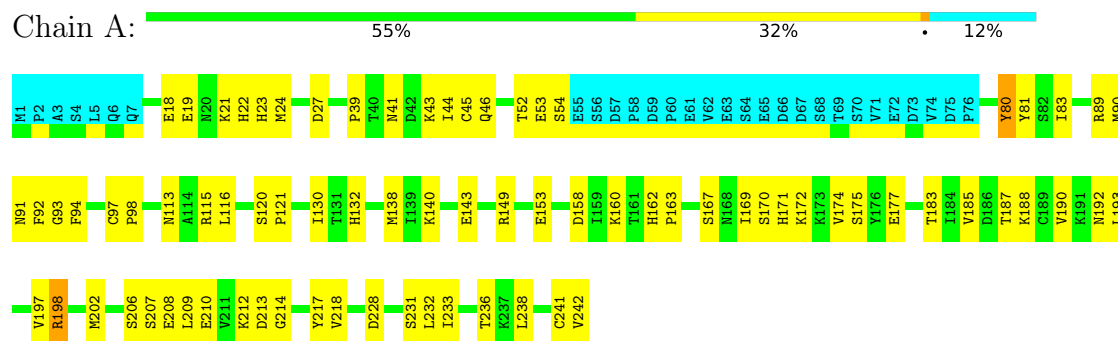
Chain	Residue	Modelled	Actual	Comment	Reference
B	45	ALA	LYS	engineered mutation	UNP P13236
B	46	ALA	ARG	engineered mutation	UNP P13236
B	48	ALA	LYS	engineered mutation	UNP P13236

4 Residue-property plots [i](#)

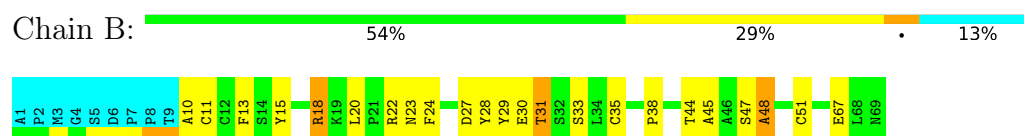
4.1 Average score per residue in the NMR ensemble

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: rabbitpox encoded CC chemokine inhibitor



- Molecule 2: Small inducible cytokine A4

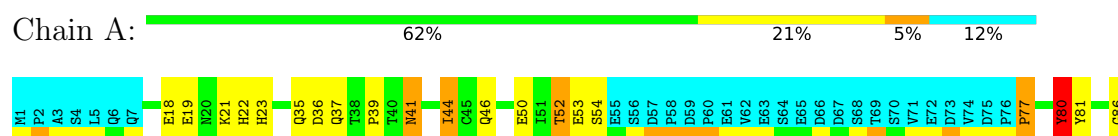


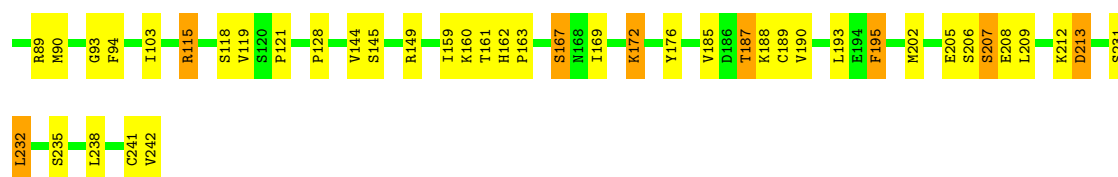
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

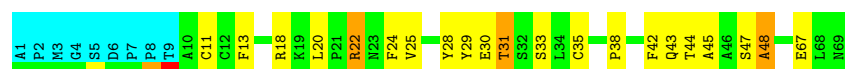
- Molecule 1: rabbitpox encoded CC chemokine inhibitor





- Molecule 2: Small inducible cytokine A4

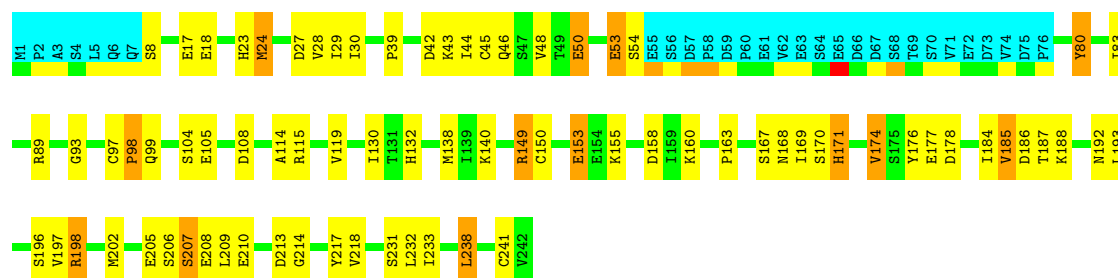
Chain B: 57% 26% 13%



4.2.2 Score per residue for model 2

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

Chain A: 56% 27% 5% 12%



- Molecule 2: Small inducible cytokine A4

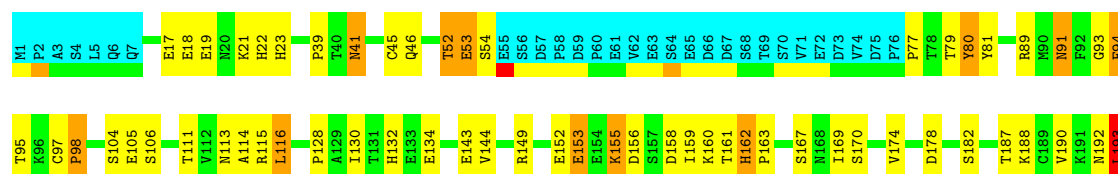
Chain B: 52% 25% 10% 13%

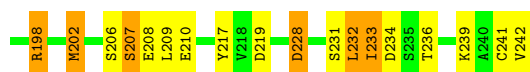


4.2.3 Score per residue for model 3

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

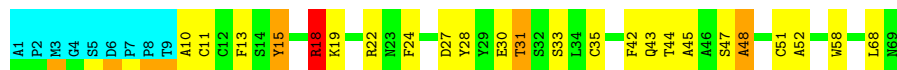
Chain A: 56% 25% 7% 12%





- Molecule 2: Small inducible cytokine A4

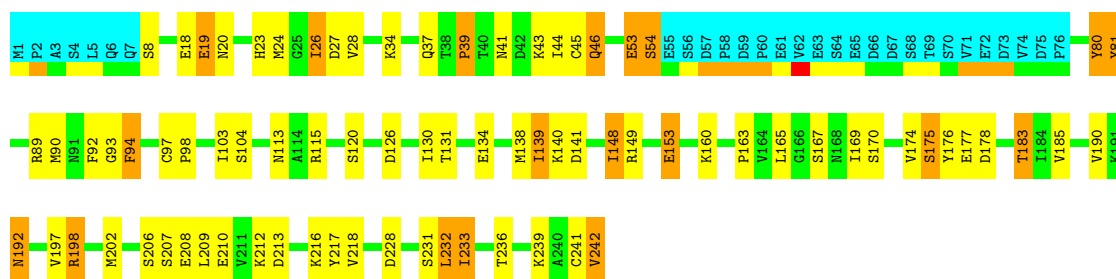
Chain B: 52% 29% 13%



4.2.4 Score per residue for model 4

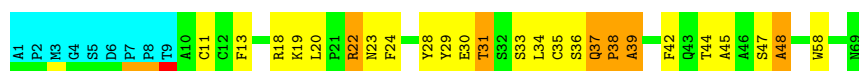
- Molecule 1: rabbitpox encoded CC chemokine inhibitor

Chain A: 55% 25% 8% 12%



- Molecule 2: Small inducible cytokine A4

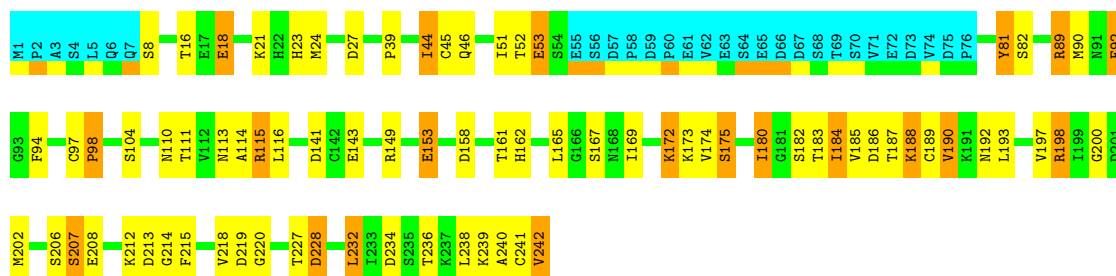
Chain B: 51% 28% 9% 13%



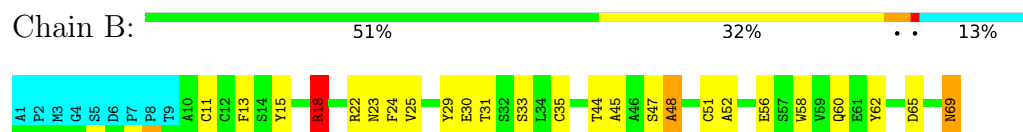
4.2.5 Score per residue for model 5

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

Chain A: 55% 24% 8% 12%

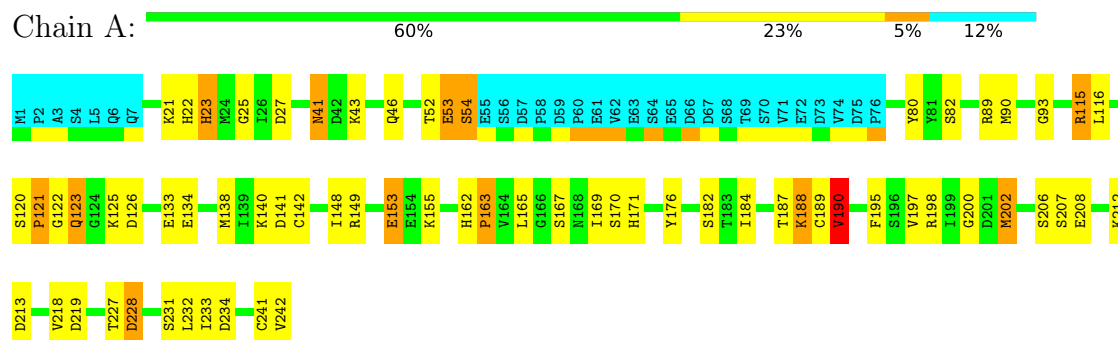


- Molecule 2: Small inducible cytokine A4

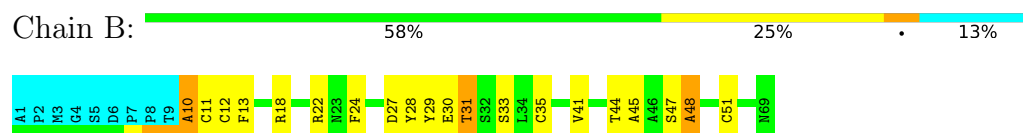


4.2.6 Score per residue for model 6

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

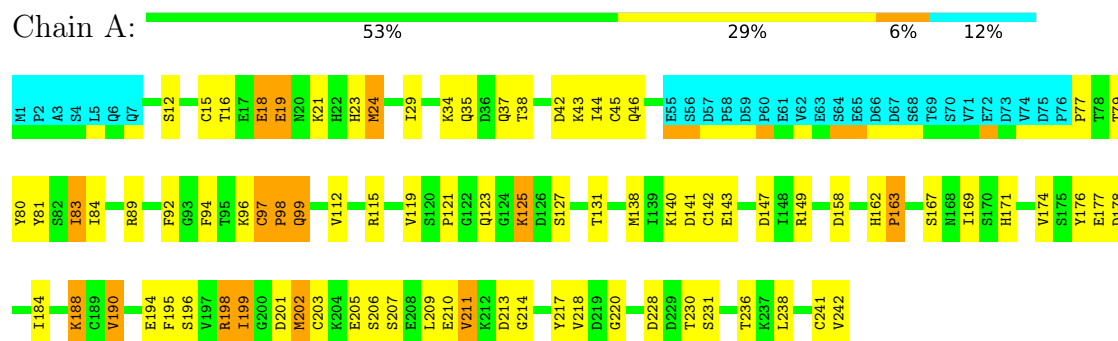


- Molecule 2: Small inducible cytokine A4

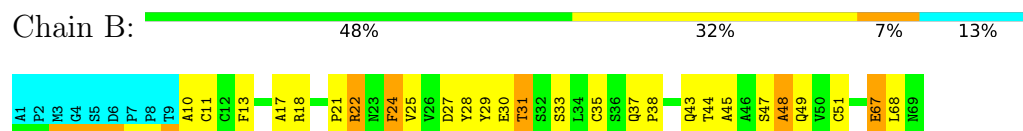


4.2.7 Score per residue for model 7

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

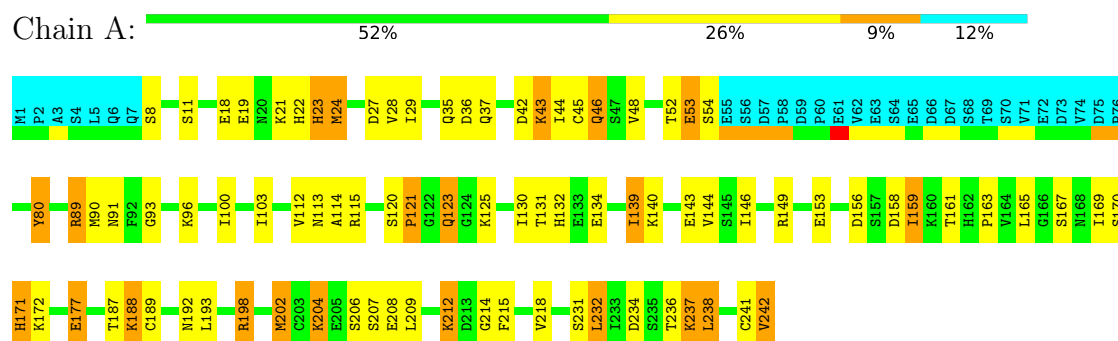


- Molecule 2: Small inducible cytokine A4

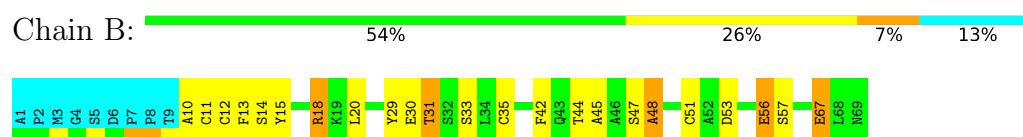


4.2.8 Score per residue for model 8

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

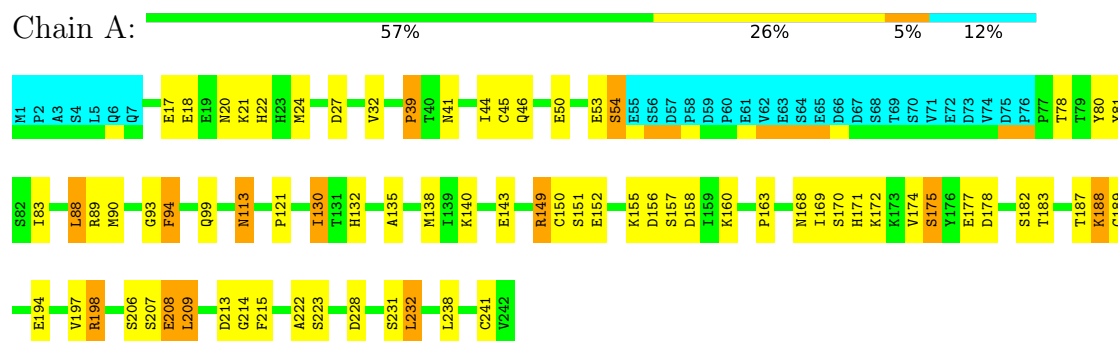


- Molecule 2: Small inducible cytokine A4

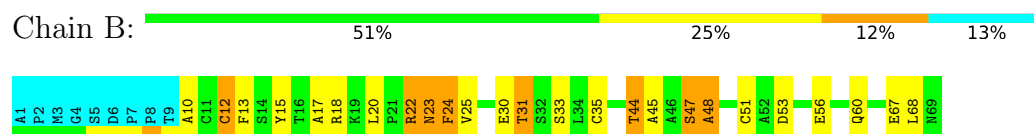


4.2.9 Score per residue for model 9

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

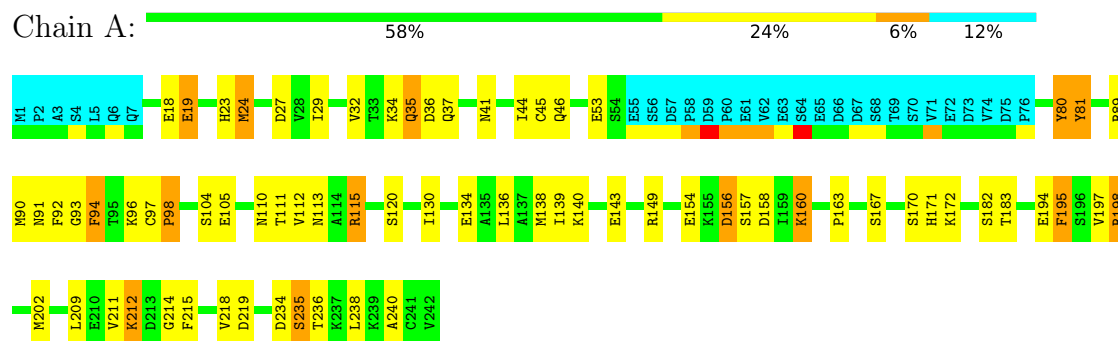


- Molecule 2: Small inducible cytokine A4

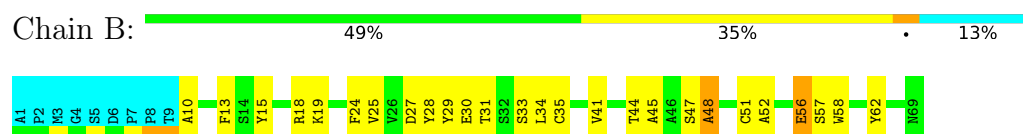


4.2.10 Score per residue for model 10

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

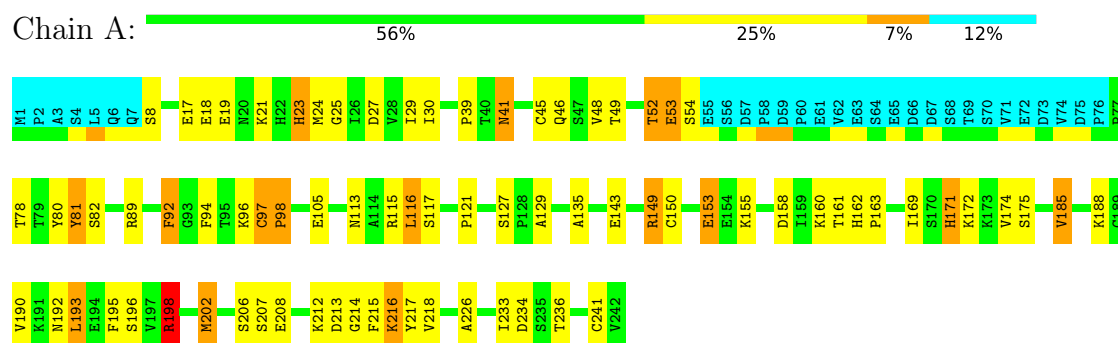


- Molecule 2: Small inducible cytokine A4

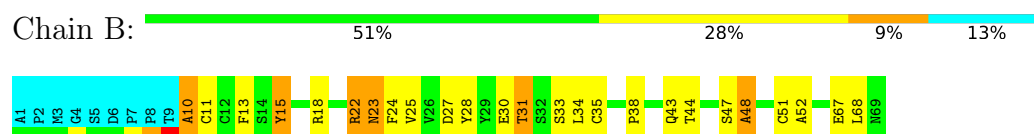


4.2.11 Score per residue for model 11

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

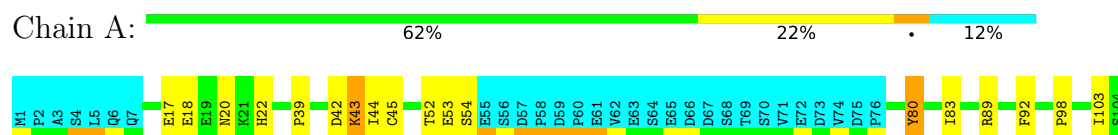


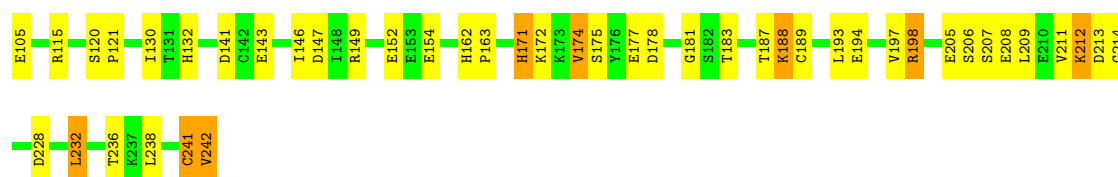
- Molecule 2: Small inducible cytokine A4



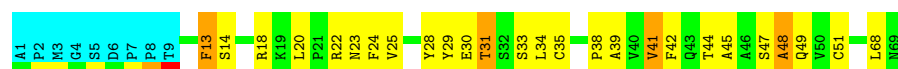
4.2.12 Score per residue for model 12

- Molecule 1: rabbitpox encoded CC chemokine inhibitor



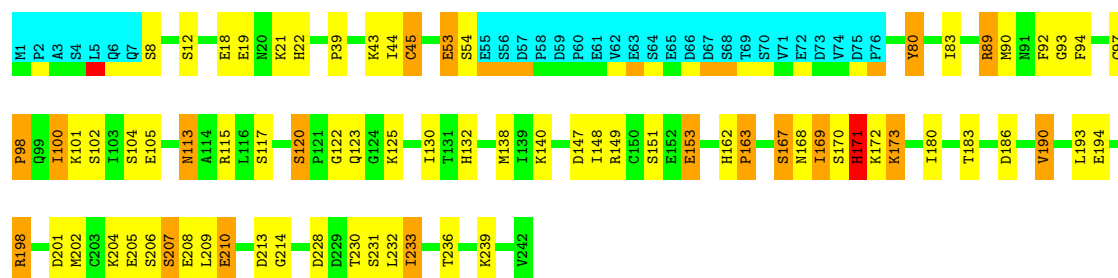


- Molecule 2: Small inducible cytokine A4

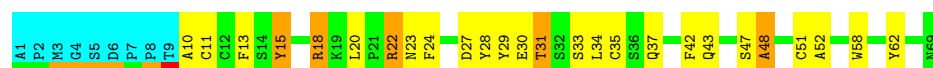


4.2.13 Score per residue for model 13

- Molecule 1: rabbitpox encoded CC chemokine inhibitor

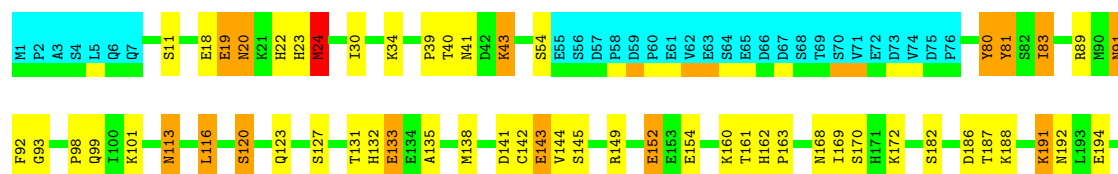


- Molecule 2: Small inducible cytokine A4



4.2.14 Score per residue for model 14

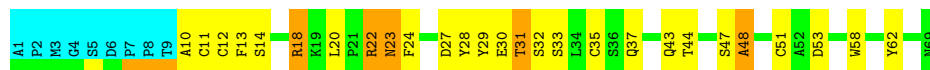
- Molecule 1: rabbitpox encoded CC chemokine inhibitor





- Molecule 2: Small inducible cytokine A4

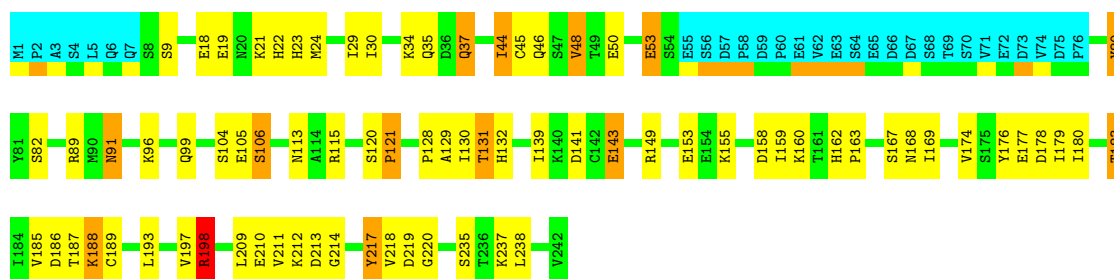
Chain B: 48% 32% 7% 13%



4.2.15 Score per residue for model 15 (medoid)

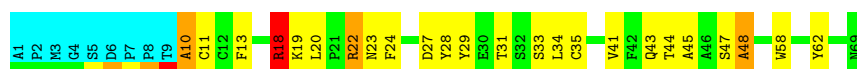
- Molecule 1: rabbitpox encoded CC chemokine inhibitor

Chain A: 56% 26% 5% 12%



- Molecule 2: Small inducible cytokine A4

Chain B: 52% 29% 13%



5 Refinement protocol and experimental data overview

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy.*

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

Software name	Classification	Version
DYNAMO	structure solution	3.1
DYNAMO	refinement	3.1

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.68±0.01	0±0/1620 (0.0± 0.0%)	0.95±0.01	0±0/2179 (0.0± 0.0%)
2	B	0.73±0.01	0±0/487 (0.0± 0.0%)	0.95±0.01	0±0/665 (0.0± 0.0%)
All	All	0.69	0/31605 (0.0%)	0.95	3/42660 (0.0%)

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	3.9±0.6
2	B	0.0±0.0	1.7±0.5
All	All	0	84

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	HIS	CA-CB-CG	-5.71	108.08	113.80	11	3

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	89	ARG	Sidechain	15
1	A	149	ARG	Sidechain	15
2	B	18	ARG	Sidechain	14
1	A	198	ARG	Sidechain	13
1	A	115	ARG	Sidechain	11
2	B	22	ARG	Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	80	TYR	Sidechain	3
1	A	81	TYR	Sidechain	2

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	1602	1571	1571	65±11
2	B	475	436	436	21±3
All	All	31155	30105	30105	1250

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:19:LYS:HZ3	2:B:58:TRP:CG	0.85	1.88	3	1
1:A:139:ILE:HD13	1:A:140:LYS:N	0.85	1.86	4	2
1:A:116:LEU:N	1:A:116:LEU:HD22	0.79	1.92	11	2
2:B:68:LEU:HD23	2:B:69:ASN:N	0.75	1.96	2	1
1:A:116:LEU:HD12	1:A:116:LEU:N	0.71	1.99	3	1
1:A:174:VAL:HG22	1:A:175:SER:H	0.70	1.46	11	2
1:A:125:LYS:HZ1	1:A:127:SER:CB	0.70	1.99	7	1
1:A:184:ILE:N	1:A:184:ILE:HD12	0.69	2.01	5	3
2:B:19:LYS:HZ1	2:B:58:TRP:CD1	0.67	2.08	4	1
1:A:81:TYR:CD2	1:A:92:PHE:CE1	0.66	2.84	11	1
1:A:160:LYS:HZ3	1:A:240:ALA:H	0.65	1.34	10	1
1:A:202:MET:HE3	1:A:202:MET:C	0.65	2.15	3	1
1:A:123:GLN:HE21	1:A:125:LYS:H	0.63	1.33	13	1
1:A:148:ILE:HD11	1:A:190:VAL:CG2	0.62	2.24	4	1
1:A:174:VAL:HG22	1:A:175:SER:N	0.62	2.09	11	3
1:A:202:MET:SD	1:A:202:MET:N	0.62	2.72	5	3
1:A:209:LEU:HD22	1:A:209:LEU:N	0.62	2.10	15	4
1:A:171:HIS:N	1:A:171:HIS:ND1	0.62	2.48	13	1
1:A:100:ILE:HD12	1:A:100:ILE:C	0.62	2.20	8	1
1:A:159:ILE:HD13	1:A:159:ILE:H	0.61	1.54	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:MET:N	1:A:24:MET:SD	0.60	2.74	2	2
1:A:81:TYR:CD1	1:A:81:TYR:N	0.60	2.70	10	3
1:A:91:ASN:N	1:A:91:ASN:HD22	0.59	1.95	3	1
2:B:43:GLN:N	2:B:43:GLN:NE2	0.59	2.51	3	1
1:A:193:LEU:C	1:A:193:LEU:HD23	0.59	2.23	12	4
1:A:160:LYS:NZ	1:A:162:HIS:NE2	0.59	2.50	11	1
1:A:195:PHE:N	1:A:195:PHE:CD1	0.59	2.69	1	2
1:A:116:LEU:N	1:A:116:LEU:CD2	0.59	2.64	11	2
1:A:193:LEU:HD12	1:A:195:PHE:CZ	0.59	2.33	11	1
1:A:113:ASN:ND2	1:A:114:ALA:N	0.58	2.50	3	2
1:A:138:MET:SD	1:A:139:ILE:N	0.58	2.76	10	1
1:A:169:ILE:C	1:A:169:ILE:HD12	0.58	2.23	14	2
1:A:81:TYR:CE2	1:A:92:PHE:CD2	0.58	2.91	14	1
1:A:81:TYR:CZ	1:A:92:PHE:CG	0.58	2.91	11	1
1:A:22:HIS:CD2	1:A:132:HIS:NE2	0.58	2.72	14	1
1:A:22:HIS:CE1	1:A:132:HIS:NE2	0.58	2.71	3	2
1:A:50:GLU:CD	1:A:50:GLU:H	0.57	2.07	2	2
1:A:182:SER:OG	2:B:51:CYS:N	0.57	2.37	9	2
1:A:23:HIS:CE1	1:A:202:MET:SD	0.57	2.98	14	1
2:B:47:SER:O	2:B:48:ALA:HB2	0.57	2.00	1	15
2:B:68:LEU:HD12	2:B:68:LEU:N	0.57	2.15	12	1
1:A:90:MET:SD	1:A:90:MET:N	0.57	2.78	4	4
1:A:159:ILE:H	1:A:159:ILE:CD1	0.56	2.12	8	1
1:A:123:GLN:NE2	1:A:125:LYS:H	0.56	1.96	13	1
1:A:172:LYS:N	1:A:198:ARG:HH12	0.56	1.97	12	1
1:A:25:GLY:N	1:A:202:MET:SD	0.56	2.78	6	2
1:A:46:GLN:NE2	1:A:155:LYS:N	0.56	2.54	15	2
1:A:20:ASN:HD22	1:A:20:ASN:N	0.56	1.98	14	1
1:A:209:LEU:HD12	1:A:209:LEU:N	0.56	2.16	3	5
1:A:92:PHE:CD1	1:A:92:PHE:C	0.56	2.84	11	2
2:B:43:GLN:NE2	2:B:44:THR:H	0.56	1.99	11	1
1:A:80:TYR:C	1:A:80:TYR:CD1	0.55	2.84	15	6
1:A:162:HIS:N	1:A:162:HIS:ND1	0.55	2.54	3	1
1:A:130:ILE:H	1:A:130:ILE:HD13	0.55	1.61	9	1
1:A:99:GLN:NE2	1:A:99:GLN:H	0.55	1.98	9	1
1:A:202:MET:HE3	1:A:202:MET:H	0.55	1.61	7	1
1:A:122:GLY:N	1:A:123:GLN:NE2	0.55	2.55	6	1
2:B:11:CYS:O	2:B:13:PHE:CE1	0.55	2.60	13	9
1:A:92:PHE:CE2	1:A:94:PHE:CD1	0.55	2.95	5	1
2:B:20:LEU:HD22	2:B:20:LEU:N	0.55	2.16	15	3
1:A:162:HIS:NE2	1:A:240:ALA:CB	0.55	2.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:TYR:CD1	1:A:81:TYR:N	0.54	2.75	1	2
1:A:190:VAL:O	1:A:190:VAL:HG13	0.54	2.03	5	2
1:A:35:GLN:NE2	1:A:37:GLN:H	0.54	2.01	10	1
1:A:45:CYS:SG	1:A:45:CYS:O	0.54	2.65	10	9
1:A:153:GLU:CD	1:A:153:GLU:H	0.54	2.11	2	3
1:A:184:ILE:N	1:A:184:ILE:CD1	0.54	2.70	5	3
1:A:22:HIS:ND1	1:A:132:HIS:CD2	0.54	2.76	3	1
1:A:123:GLN:OE1	1:A:123:GLN:N	0.54	2.40	13	2
1:A:19:GLU:H	1:A:19:GLU:CD	0.54	2.10	8	2
1:A:209:LEU:N	1:A:209:LEU:CD2	0.54	2.70	14	4
1:A:23:HIS:N	1:A:23:HIS:ND1	0.54	2.56	8	1
1:A:113:ASN:ND2	1:A:113:ASN:H	0.54	2.00	13	2
2:B:34:LEU:N	2:B:34:LEU:CD1	0.54	2.70	10	2
2:B:24:PHE:CD1	2:B:24:PHE:N	0.54	2.76	3	7
1:A:233:ILE:C	1:A:233:ILE:HD12	0.54	2.27	2	1
2:B:19:LYS:HZ3	2:B:58:TRP:CD1	0.54	2.21	3	1
2:B:19:LYS:HZ1	2:B:58:TRP:CG	0.54	2.21	4	1
1:A:99:GLN:H	1:A:99:GLN:CD	0.54	2.10	7	2
1:A:205:GLU:H	1:A:205:GLU:CD	0.54	2.11	1	3
1:A:94:PHE:C	1:A:94:PHE:CD1	0.54	2.86	10	7
1:A:202:MET:SD	1:A:203:CYS:SG	0.54	3.06	7	1
1:A:187:THR:O	1:A:189:CYS:N	0.53	2.41	6	6
1:A:139:ILE:HD13	1:A:139:ILE:C	0.53	2.28	8	2
1:A:81:TYR:CE2	1:A:92:PHE:CE1	0.53	2.96	11	1
1:A:208:GLU:H	1:A:208:GLU:CD	0.53	2.11	9	1
1:A:123:GLN:N	1:A:123:GLN:CD	0.53	2.66	6	3
1:A:233:ILE:H	1:A:233:ILE:HD13	0.53	1.63	3	1
2:B:44:THR:OG1	2:B:45:ALA:N	0.53	2.39	7	12
1:A:16:THR:H	1:A:23:HIS:CE1	0.53	2.22	5	1
2:B:68:LEU:CD2	2:B:69:ASN:N	0.53	2.70	2	1
1:A:161:THR:O	1:A:161:THR:HG22	0.53	2.03	3	6
2:B:56:GLU:OE1	2:B:57:SER:N	0.53	2.42	8	2
1:A:46:GLN:HE21	1:A:46:GLN:N	0.53	2.01	4	1
1:A:165:LEU:HD12	1:A:165:LEU:N	0.52	2.19	5	3
1:A:121:PRO:C	1:A:123:GLN:NE2	0.52	2.67	6	1
1:A:192:ASN:ND2	1:A:217:TYR:O	0.52	2.42	3	1
2:B:37:GLN:N	2:B:38:PRO:CD	0.52	2.72	4	1
1:A:29:ILE:HD11	1:A:171:HIS:NE2	0.52	2.19	7	1
1:A:210:GLU:C	1:A:211:VAL:HG12	0.52	2.29	7	1
1:A:81:TYR:CE2	1:A:92:PHE:CZ	0.52	2.96	11	1
1:A:23:HIS:CE1	1:A:121:PRO:CG	0.52	2.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:34:LEU:CD2	2:B:34:LEU:N	0.52	2.73	15	5
1:A:113:ASN:ND2	1:A:114:ALA:H	0.52	2.03	3	2
1:A:233:ILE:CD1	1:A:233:ILE:N	0.52	2.72	3	1
1:A:83:ILE:HG23	1:A:83:ILE:O	0.52	2.05	14	4
1:A:185:VAL:O	1:A:185:VAL:HG23	0.52	2.05	5	5
1:A:165:LEU:N	1:A:165:LEU:CD1	0.52	2.72	5	2
1:A:122:GLY:N	1:A:123:GLN:HE22	0.52	2.03	6	1
2:B:20:LEU:N	2:B:20:LEU:CD2	0.52	2.73	8	4
1:A:206:SER:C	1:A:207:SER:HG	0.52	2.12	14	1
1:A:144:VAL:HG12	1:A:145:SER:N	0.52	2.19	1	2
1:A:206:SER:O	1:A:208:GLU:N	0.52	2.42	14	11
1:A:46:GLN:HE21	1:A:46:GLN:CA	0.52	2.18	4	1
1:A:218:VAL:C	1:A:220:GLY:H	0.52	2.13	15	3
1:A:123:GLN:HE21	1:A:125:LYS:N	0.52	2.03	13	1
2:B:20:LEU:HD12	2:B:24:PHE:CD2	0.52	2.40	13	1
1:A:133:GLU:CD	1:A:133:GLU:H	0.52	2.13	6	1
1:A:183:THR:O	2:B:13:PHE:CZ	0.52	2.63	12	1
1:A:99:GLN:CD	1:A:99:GLN:N	0.51	2.69	7	2
1:A:80:TYR:CE1	1:A:91:ASN:OD1	0.51	2.64	14	2
1:A:187:THR:C	1:A:189:CYS:N	0.51	2.66	6	6
1:A:171:HIS:NE2	1:A:196:SER:OG	0.51	2.44	2	1
1:A:197:VAL:HG22	1:A:198:ARG:N	0.51	2.20	2	4
1:A:159:ILE:HG22	1:A:160:LYS:N	0.51	2.20	3	2
1:A:192:ASN:CG	1:A:193:LEU:N	0.51	2.68	3	1
1:A:23:HIS:NE2	1:A:127:SER:OG	0.51	2.43	14	1
1:A:35:GLN:CD	1:A:36:ASP:N	0.51	2.69	1	2
1:A:131:THR:HG22	1:A:132:HIS:N	0.51	2.20	8	2
1:A:113:ASN:CG	1:A:233:ILE:HD11	0.51	2.31	4	1
1:A:80:TYR:CD2	1:A:92:PHE:O	0.51	2.64	7	4
1:A:217:TYR:C	1:A:217:TYR:CD1	0.51	2.88	15	1
2:B:29:TYR:CG	2:B:30:GLU:N	0.51	2.79	8	4
1:A:26:ILE:HD13	1:A:27:ASP:N	0.51	2.21	4	1
1:A:53:GLU:CD	2:B:24:PHE:CE1	0.51	2.89	4	1
1:A:53:GLU:O	1:A:54:SER:CB	0.51	2.58	9	2
1:A:23:HIS:CD2	1:A:127:SER:OG	0.51	2.64	11	2
2:B:68:LEU:N	2:B:68:LEU:CD1	0.51	2.73	12	1
1:A:132:HIS:CD2	1:A:132:HIS:N	0.51	2.77	3	2
1:A:19:GLU:N	1:A:19:GLU:CD	0.51	2.69	4	3
1:A:165:LEU:N	1:A:165:LEU:CD2	0.51	2.74	8	1
1:A:116:LEU:HD22	1:A:116:LEU:H	0.51	1.65	11	1
1:A:45:CYS:SG	1:A:158:ASP:O	0.51	2.69	10	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:TYR:CD1	2:B:15:TYR:N	0.51	2.79	10	4
1:A:24:MET:HE1	1:A:130:ILE:H	0.51	1.66	4	1
1:A:81:TYR:CD1	1:A:81:TYR:O	0.51	2.64	5	1
1:A:52:THR:O	1:A:54:SER:N	0.51	2.44	11	1
1:A:198:ARG:NH1	1:A:210:GLU:OE2	0.51	2.44	13	1
1:A:153:GLU:N	1:A:153:GLU:OE2	0.51	2.44	4	2
1:A:136:LEU:O	1:A:140:LYS:NZ	0.51	2.44	10	1
1:A:172:LYS:O	1:A:198:ARG:NH2	0.51	2.43	12	1
1:A:22:HIS:NE2	1:A:132:HIS:NE2	0.51	2.58	14	1
1:A:207:SER:N	1:A:210:GLU:OE1	0.50	2.44	2	3
1:A:79:THR:OG1	1:A:94:PHE:CE2	0.50	2.64	7	2
1:A:34:LYS:CB	1:A:34:LYS:NZ	0.50	2.75	4	1
1:A:48:VAL:CG1	1:A:241:CYS:SG	0.50	2.99	11	1
2:B:56:GLU:O	2:B:60:GLN:NE2	0.50	2.45	5	1
1:A:123:GLN:NE2	1:A:125:LYS:O	0.50	2.44	13	2
1:A:130:ILE:CD1	1:A:130:ILE:N	0.50	2.74	9	1
2:B:49:GLN:O	2:B:49:GLN:NE2	0.50	2.45	12	1
1:A:114:ALA:H	1:A:115:ARG:NH2	0.50	2.04	2	1
1:A:190:VAL:O	1:A:190:VAL:HG23	0.50	2.06	3	2
1:A:22:HIS:CD2	1:A:132:HIS:CD2	0.50	2.99	14	1
1:A:91:ASN:HD22	1:A:91:ASN:C	0.50	2.13	15	2
1:A:174:VAL:O	1:A:176:TYR:CE1	0.50	2.64	15	1
1:A:23:HIS:ND1	1:A:128:PRO:O	0.50	2.44	1	1
1:A:30:ILE:HG23	1:A:30:ILE:O	0.50	2.07	2	2
1:A:24:MET:SD	1:A:24:MET:O	0.50	2.70	8	2
1:A:53:GLU:OE2	1:A:78:THR:N	0.50	2.44	11	1
1:A:153:GLU:CD	1:A:153:GLU:N	0.50	2.70	11	4
1:A:53:GLU:OE1	1:A:54:SER:N	0.50	2.44	3	1
1:A:141:ASP:OD2	2:B:18:ARG:NE	0.50	2.45	4	1
1:A:17:GLU:CD	1:A:17:GLU:N	0.50	2.70	12	4
1:A:153:GLU:N	1:A:153:GLU:OE1	0.50	2.44	13	3
1:A:172:LYS:CB	1:A:172:LYS:NZ	0.50	2.75	5	1
1:A:23:HIS:CE1	1:A:127:SER:OG	0.50	2.65	14	2
1:A:159:ILE:CD1	1:A:159:ILE:N	0.50	2.74	8	1
1:A:53:GLU:CG	1:A:53:GLU:O	0.50	2.59	11	1
2:B:11:CYS:O	2:B:13:PHE:CE2	0.50	2.64	11	1
1:A:183:THR:OG1	2:B:13:PHE:CE2	0.50	2.62	12	1
1:A:212:LYS:NZ	1:A:227:THR:O	0.50	2.45	14	1
1:A:29:ILE:CD1	1:A:29:ILE:N	0.50	2.74	2	1
1:A:42:ASP:O	1:A:44:ILE:N	0.50	2.45	7	4
1:A:50:GLU:CD	1:A:50:GLU:N	0.50	2.70	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:GLU:CD	1:A:178:ASP:N	0.50	2.70	15	5
1:A:210:GLU:N	1:A:210:GLU:OE1	0.50	2.45	14	2
1:A:204:LYS:CB	1:A:204:LYS:NZ	0.50	2.75	8	1
1:A:105:GLU:N	1:A:105:GLU:OE1	0.50	2.44	10	1
1:A:192:ASN:ND2	1:A:194:GLU:OE1	0.50	2.45	14	1
1:A:21:LYS:NZ	1:A:129:ALA:C	0.50	2.70	15	2
1:A:40:THR:O	1:A:41:ASN:ND2	0.50	2.45	14	1
2:B:20:LEU:N	2:B:20:LEU:HD12	0.50	2.20	9	4
1:A:183:THR:O	2:B:13:PHE:CE2	0.50	2.64	4	1
2:B:58:TRP:O	2:B:62:TYR:CD1	0.50	2.65	14	5
2:B:22:ARG:CG	2:B:22:ARG:HH11	0.50	2.20	7	1
1:A:49:THR:OG1	1:A:82:SER:N	0.50	2.45	11	1
1:A:27:ASP:OD1	1:A:28:VAL:N	0.49	2.45	4	3
1:A:210:GLU:OE1	1:A:210:GLU:N	0.49	2.44	2	1
1:A:214:GLY:C	1:A:215:PHE:CD1	0.49	2.90	10	2
1:A:242:VAL:HG22	1:A:242:VAL:O	0.49	2.07	7	3
1:A:170:SER:O	1:A:198:ARG:NH1	0.49	2.45	6	3
1:A:213:ASP:OD1	1:A:214:GLY:N	0.49	2.45	13	7
2:B:20:LEU:CD1	2:B:20:LEU:N	0.49	2.75	4	1
1:A:177:GLU:OE2	1:A:178:ASP:N	0.49	2.45	7	2
1:A:21:LYS:O	1:A:22:HIS:CD2	0.49	2.65	8	1
1:A:20:ASN:OD1	1:A:132:HIS:CG	0.49	2.66	12	2
2:B:29:TYR:CE2	2:B:30:GLU:O	0.49	2.65	6	6
2:B:64:TYR:CE1	2:B:67:GLU:OE2	0.49	2.66	2	1
1:A:192:ASN:C	1:A:192:ASN:ND2	0.49	2.71	4	1
1:A:11:SER:OG	1:A:23:HIS:CD2	0.49	2.66	8	1
1:A:11:SER:OG	1:A:23:HIS:NE2	0.49	2.46	8	1
2:B:15:TYR:CD2	2:B:53:ASP:OD2	0.49	2.66	8	1
1:A:172:LYS:O	1:A:198:ARG:NH1	0.49	2.45	12	1
1:A:21:LYS:O	1:A:22:HIS:CG	0.49	2.65	1	3
2:B:28:TYR:O	2:B:29:TYR:CD2	0.49	2.66	1	1
1:A:113:ASN:HD22	1:A:114:ALA:H	0.49	1.47	3	1
1:A:43:LYS:N	1:A:43:LYS:CD	0.49	2.76	14	2
1:A:143:GLU:N	1:A:143:GLU:OE1	0.49	2.45	15	1
1:A:29:ILE:N	1:A:29:ILE:HD12	0.49	2.22	2	1
1:A:46:GLN:OE1	1:A:155:LYS:N	0.49	2.46	2	1
1:A:197:VAL:CG2	1:A:198:ARG:N	0.49	2.76	2	4
1:A:104:SER:OG	1:A:105:GLU:N	0.49	2.46	3	2
1:A:152:GLU:OE1	1:A:152:GLU:N	0.49	2.45	3	1
1:A:24:MET:SD	1:A:130:ILE:HG22	0.49	2.48	10	1
1:A:143:GLU:CD	2:B:18:ARG:HE	0.49	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ILE:CD1	1:A:44:ILE:N	0.49	2.76	1	1
2:B:33:SER:C	2:B:35:CYS:N	0.49	2.70	11	15
1:A:162:HIS:O	1:A:162:HIS:CD2	0.49	2.66	5	1
1:A:99:GLN:OE1	1:A:101:LYS:NZ	0.49	2.46	14	1
1:A:37:GLN:N	1:A:37:GLN:OE1	0.49	2.45	15	1
1:A:209:LEU:N	1:A:209:LEU:CD1	0.49	2.75	3	4
2:B:68:LEU:HD23	2:B:68:LEU:C	0.49	2.33	2	1
1:A:39:PRO:O	1:A:41:ASN:ND2	0.49	2.46	9	2
1:A:34:LYS:NZ	1:A:110:ASN:C	0.49	2.71	10	1
2:B:30:GLU:CD	2:B:30:GLU:N	0.49	2.71	13	1
1:A:48:VAL:CG2	1:A:241:CYS:SG	0.49	3.00	2	1
1:A:174:VAL:O	1:A:175:SER:C	0.49	2.55	4	4
1:A:41:ASN:ND2	1:A:41:ASN:N	0.49	2.60	6	1
1:A:133:GLU:CD	1:A:133:GLU:N	0.49	2.71	6	2
1:A:194:GLU:N	1:A:194:GLU:CD	0.49	2.71	13	5
2:B:48:ALA:C	2:B:49:GLN:NE2	0.49	2.70	7	1
1:A:123:GLN:CD	1:A:125:LYS:H	0.49	2.15	8	1
2:B:24:PHE:O	2:B:24:PHE:CD2	0.49	2.66	11	1
1:A:24:MET:SD	1:A:24:MET:C	0.49	2.96	14	1
1:A:91:ASN:C	1:A:91:ASN:ND2	0.49	2.69	14	2
1:A:21:LYS:C	1:A:22:HIS:CG	0.49	2.91	15	4
1:A:231:SER:C	1:A:233:ILE:N	0.49	2.70	2	4
2:B:15:TYR:CE2	2:B:53:ASP:OD1	0.49	2.65	2	2
1:A:46:GLN:NE2	1:A:155:LYS:O	0.49	2.45	6	4
1:A:152:GLU:N	1:A:152:GLU:CD	0.49	2.71	3	1
2:B:12:CYS:SG	2:B:14:SER:O	0.49	2.70	8	1
1:A:106:SER:OG	1:A:113:ASN:ND2	0.49	2.45	15	1
1:A:205:GLU:CD	1:A:205:GLU:N	0.49	2.71	7	3
1:A:210:GLU:N	1:A:210:GLU:CD	0.49	2.70	3	3
1:A:231:SER:O	1:A:233:ILE:N	0.49	2.46	2	4
1:A:37:GLN:CD	1:A:37:GLN:N	0.49	2.71	4	1
1:A:41:ASN:ND2	1:A:41:ASN:O	0.49	2.46	6	1
2:B:15:TYR:CE2	2:B:53:ASP:OD2	0.49	2.66	8	1
1:A:53:GLU:OE1	2:B:24:PHE:CZ	0.49	2.66	11	1
2:B:28:TYR:C	2:B:29:TYR:CD1	0.49	2.91	15	1
2:B:34:LEU:N	2:B:34:LEU:HD22	0.48	2.23	4	5
2:B:51:CYS:SG	2:B:52:ALA:N	0.48	2.86	10	5
1:A:44:ILE:HD12	1:A:44:ILE:O	0.48	2.07	5	2
1:A:113:ASN:N	1:A:113:ASN:ND2	0.48	2.61	9	1
1:A:80:TYR:CD1	1:A:80:TYR:C	0.48	2.90	13	1
1:A:113:ASN:ND2	1:A:113:ASN:N	0.48	2.60	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:GLU:N	1:A:18:GLU:CD	0.48	2.71	15	1
1:A:99:GLN:N	1:A:99:GLN:CD	0.48	2.71	2	2
1:A:183:THR:O	2:B:13:PHE:CD1	0.48	2.66	5	2
1:A:238:LEU:CD1	1:A:238:LEU:N	0.48	2.76	7	2
1:A:113:ASN:CG	1:A:114:ALA:N	0.48	2.71	8	1
2:B:47:SER:O	2:B:48:ALA:CB	0.48	2.62	2	15
2:B:15:TYR:CD2	2:B:53:ASP:OD1	0.48	2.65	9	2
1:A:214:GLY:O	1:A:215:PHE:CD1	0.48	2.66	11	3
1:A:115:ARG:NH2	1:A:235:SER:OG	0.48	2.47	1	1
1:A:153:GLU:N	1:A:153:GLU:CD	0.48	2.71	3	2
1:A:123:GLN:NE2	1:A:123:GLN:N	0.48	2.61	6	1
1:A:41:ASN:C	1:A:41:ASN:HD22	0.48	2.17	3	1
1:A:53:GLU:OE1	2:B:24:PHE:CE1	0.48	2.67	15	3
1:A:46:GLN:O	1:A:46:GLN:NE2	0.48	2.46	1	2
2:B:28:TYR:O	2:B:29:TYR:CG	0.48	2.66	13	4
1:A:46:GLN:HE22	1:A:156:ASP:C	0.48	2.16	3	1
1:A:183:THR:OG1	2:B:13:PHE:CE1	0.48	2.62	4	2
1:A:156:ASP:CG	1:A:157:SER:N	0.48	2.71	10	1
2:B:43:GLN:CG	2:B:44:THR:N	0.48	2.77	15	4
1:A:29:ILE:CG1	1:A:115:ARG:HE	0.48	2.21	8	1
1:A:35:GLN:C	1:A:37:GLN:N	0.48	2.72	8	2
2:B:19:LYS:HZ2	2:B:58:TRP:CD1	0.48	2.27	10	1
1:A:131:THR:OG1	1:A:132:HIS:N	0.48	2.47	15	1
2:B:47:SER:OG	2:B:48:ALA:N	0.48	2.47	1	2
2:B:22:ARG:C	2:B:24:PHE:H	0.48	2.17	14	5
1:A:215:PHE:CD1	1:A:215:PHE:N	0.48	2.81	10	1
1:A:154:GLU:CD	1:A:154:GLU:N	0.48	2.71	14	1
1:A:44:ILE:N	1:A:44:ILE:HD13	0.48	2.24	1	1
2:B:15:TYR:CZ	2:B:53:ASP:OD1	0.48	2.67	2	1
1:A:219:ASP:N	1:A:219:ASP:OD1	0.48	2.45	6	2
1:A:115:ARG:NH1	1:A:235:SER:OG	0.48	2.47	10	1
1:A:159:ILE:C	1:A:159:ILE:HD12	0.48	2.34	1	1
2:B:28:TYR:C	2:B:29:TYR:CD2	0.48	2.92	1	1
1:A:18:GLU:O	1:A:21:LYS:N	0.48	2.47	3	1
2:B:29:TYR:CD2	2:B:30:GLU:O	0.48	2.67	8	5
2:B:20:LEU:N	2:B:20:LEU:HD22	0.48	2.24	8	1
1:A:213:ASP:CG	1:A:214:GLY:N	0.48	2.72	15	2
1:A:211:VAL:CG1	1:A:212:LYS:N	0.48	2.76	10	2
1:A:159:ILE:CG2	1:A:160:LYS:N	0.47	2.77	3	2
1:A:89:ARG:CZ	1:A:91:ASN:HD21	0.47	2.21	8	1
1:A:41:ASN:ND2	1:A:154:GLU:OE1	0.47	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:VAL:HG21	1:A:217:TYR:CE2	0.47	2.43	15	1
2:B:12:CYS:SG	2:B:31:THR:CG2	0.47	3.02	6	3
1:A:113:ASN:N	1:A:113:ASN:HD22	0.47	2.07	13	2
1:A:174:VAL:HG13	1:A:175:SER:N	0.47	2.24	12	1
1:A:228:ASP:CG	1:A:230:THR:HG1	0.47	2.16	13	1
2:B:38:PRO:O	2:B:39:ALA:HB2	0.47	2.09	2	3
1:A:18:GLU:O	1:A:20:ASN:N	0.47	2.46	4	1
1:A:126:ASP:N	1:A:126:ASP:OD1	0.47	2.45	4	2
1:A:212:LYS:CG	1:A:213:ASP:N	0.47	2.78	6	2
1:A:123:GLN:NE2	1:A:125:LYS:C	0.47	2.73	8	1
1:A:105:GLU:N	1:A:105:GLU:CD	0.47	2.71	10	1
1:A:23:HIS:CE1	1:A:127:SER:C	0.47	2.92	11	1
1:A:120:SER:CB	1:A:168:ASN:ND2	0.47	2.78	14	1
1:A:177:GLU:CD	1:A:178:ASP:H	0.47	2.16	15	1
2:B:42:PHE:CD1	2:B:42:PHE:C	0.47	2.92	4	5
2:B:42:PHE:C	2:B:43:GLN:NE2	0.47	2.73	3	1
2:B:14:SER:O	2:B:51:CYS:SG	0.47	2.72	8	1
1:A:160:LYS:NZ	1:A:162:HIS:CD2	0.47	2.82	11	1
1:A:41:ASN:C	1:A:41:ASN:ND2	0.47	2.72	3	1
1:A:182:SER:OG	2:B:51:CYS:SG	0.47	2.73	14	2
1:A:156:ASP:OD1	1:A:156:ASP:N	0.47	2.45	8	1
1:A:159:ILE:HD13	1:A:159:ILE:N	0.47	2.23	8	1
1:A:218:VAL:O	1:A:218:VAL:HG23	0.47	2.08	8	2
1:A:83:ILE:HD11	1:A:241:CYS:SG	0.47	2.49	12	1
1:A:23:HIS:CE1	1:A:121:PRO:CD	0.47	2.98	15	1
1:A:81:TYR:CE2	1:A:92:PHE:CG	0.47	3.02	4	2
1:A:113:ASN:OD1	1:A:113:ASN:N	0.47	2.48	10	1
1:A:24:MET:O	1:A:202:MET:SD	0.47	2.73	14	1
1:A:18:GLU:O	1:A:19:GLU:C	0.47	2.57	7	8
1:A:46:GLN:NE2	1:A:153:GLU:O	0.47	2.48	15	4
1:A:116:LEU:N	1:A:116:LEU:CD1	0.47	2.71	3	1
1:A:134:GLU:O	1:A:138:MET:N	0.47	2.47	4	1
1:A:23:HIS:CG	1:A:23:HIS:O	0.47	2.65	7	1
1:A:96:LYS:O	1:A:138:MET:SD	0.47	2.73	7	1
1:A:171:HIS:ND1	1:A:171:HIS:N	0.47	2.61	8	2
1:A:167:SER:O	1:A:202:MET:SD	0.47	2.72	10	1
1:A:144:VAL:CG1	1:A:145:SER:N	0.47	2.78	1	2
1:A:95:THR:HG21	2:B:18:ARG:CZ	0.47	2.40	3	1
1:A:134:GLU:O	1:A:138:MET:SD	0.47	2.72	6	1
1:A:21:LYS:C	1:A:22:HIS:ND1	0.47	2.73	13	1
1:A:174:VAL:O	1:A:176:TYR:CD1	0.47	2.68	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:SER:C	1:A:169:ILE:H	0.47	2.18	15	9
1:A:134:GLU:CD	1:A:134:GLU:N	0.47	2.72	8	2
1:A:120:SER:OG	1:A:168:ASN:ND2	0.47	2.48	15	1
1:A:155:LYS:N	1:A:155:LYS:CD	0.47	2.78	9	2
1:A:23:HIS:O	1:A:202:MET:SD	0.46	2.73	8	4
1:A:192:ASN:OD1	1:A:193:LEU:N	0.46	2.48	5	3
1:A:113:ASN:ND2	1:A:233:ILE:HD11	0.46	2.25	4	1
1:A:18:GLU:O	1:A:21:LYS:NZ	0.46	2.45	5	1
1:A:174:VAL:CG2	1:A:175:SER:H	0.46	2.20	11	2
1:A:35:GLN:CD	1:A:36:ASP:H	0.46	2.18	10	1
1:A:113:ASN:CG	1:A:233:ILE:HD12	0.46	2.35	11	1
1:A:168:ASN:O	1:A:168:ASN:ND2	0.46	2.47	13	1
1:A:218:VAL:HG13	1:A:218:VAL:O	0.46	2.10	6	4
1:A:238:LEU:HD12	1:A:238:LEU:O	0.46	2.10	14	3
1:A:232:LEU:O	1:A:232:LEU:HD23	0.46	2.11	3	3
1:A:29:ILE:HD12	1:A:29:ILE:N	0.46	2.25	10	1
1:A:200:GLY:O	1:A:202:MET:SD	0.46	2.73	6	2
1:A:143:GLU:CD	2:B:17:ALA:H	0.46	2.16	9	2
1:A:184:ILE:O	1:A:184:ILE:HG23	0.46	2.10	7	1
1:A:53:GLU:CG	1:A:78:THR:H	0.46	2.22	9	1
2:B:13:PHE:CD1	2:B:13:PHE:N	0.46	2.83	8	5
1:A:150:CYS:SG	1:A:186:ASP:OD2	0.46	2.74	2	1
1:A:104:SER:OG	1:A:239:LYS:N	0.46	2.49	5	2
1:A:143:GLU:OE2	1:A:144:VAL:N	0.46	2.49	8	1
2:B:20:LEU:N	2:B:20:LEU:CD1	0.46	2.78	9	2
1:A:196:SER:O	1:A:198:ARG:NH1	0.46	2.48	11	1
1:A:241:CYS:C	1:A:242:VAL:HG13	0.46	2.35	12	1
1:A:170:SER:C	1:A:172:LYS:H	0.46	2.18	13	2
1:A:238:LEU:CD2	1:A:238:LEU:N	0.46	2.78	10	2
1:A:23:HIS:CE1	1:A:202:MET:CE	0.46	2.98	4	1
1:A:80:TYR:HH	1:A:91:ASN:CG	0.46	2.18	8	1
1:A:196:SER:OG	1:A:198:ARG:NH1	0.46	2.49	11	1
1:A:53:GLU:OE1	1:A:53:GLU:N	0.46	2.49	8	1
1:A:183:THR:OG1	2:B:13:PHE:CD2	0.46	2.68	12	1
1:A:119:VAL:O	1:A:202:MET:CE	0.46	2.64	2	1
1:A:141:ASP:CG	2:B:18:ARG:HE	0.46	2.18	5	1
1:A:201:ASP:N	1:A:201:ASP:OD1	0.46	2.48	7	1
1:A:89:ARG:NH2	1:A:151:SER:OG	0.46	2.48	13	1
1:A:113:ASN:H	1:A:113:ASN:HD22	0.46	1.53	13	1
2:B:53:ASP:N	2:B:53:ASP:OD1	0.46	2.49	14	1
1:A:177:GLU:OE1	1:A:178:ASP:N	0.46	2.49	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:TYR:CE1	2:B:13:PHE:CE2	0.46	3.03	7	1
1:A:237:LYS:NZ	1:A:237:LYS:CB	0.46	2.78	8	1
1:A:202:MET:SD	1:A:202:MET:C	0.46	2.99	7	1
1:A:80:TYR:CE1	2:B:47:SER:O	0.45	2.69	8	1
1:A:100:ILE:C	1:A:100:ILE:CD1	0.45	2.90	8	2
1:A:17:GLU:CD	1:A:17:GLU:H	0.45	2.18	12	1
1:A:234:ASP:C	1:A:236:THR:H	0.45	2.20	10	3
1:A:174:VAL:CG2	1:A:175:SER:N	0.45	2.78	11	2
1:A:27:ASP:CG	1:A:171:HIS:HE2	0.45	2.20	6	1
1:A:52:THR:O	1:A:53:GLU:C	0.45	2.60	8	1
1:A:241:CYS:SG	1:A:241:CYS:O	0.45	2.74	9	1
1:A:241:CYS:O	1:A:242:VAL:OXT	0.45	2.34	12	5
2:B:22:ARG:O	2:B:25:VAL:N	0.45	2.49	12	3
1:A:149:ARG:CG	1:A:150:CYS:N	0.45	2.79	9	3
1:A:100:ILE:O	1:A:100:ILE:HG23	0.45	2.12	13	1
1:A:176:TYR:CD1	1:A:176:TYR:O	0.45	2.69	2	3
1:A:83:ILE:O	1:A:83:ILE:CG2	0.45	2.64	7	2
1:A:130:ILE:HD13	1:A:130:ILE:N	0.45	2.25	9	1
1:A:160:LYS:NZ	1:A:162:HIS:CE1	0.45	2.85	11	1
1:A:45:CYS:SG	1:A:105:GLU:CG	0.45	3.04	12	1
1:A:207:SER:OG	1:A:208:GLU:N	0.45	2.49	1	1
1:A:193:LEU:C	1:A:193:LEU:CD2	0.45	2.90	12	2
1:A:90:MET:HE2	1:A:92:PHE:CZ	0.45	2.46	13	1
1:A:46:GLN:NE2	1:A:156:ASP:C	0.45	2.74	3	1
2:B:43:GLN:N	2:B:43:GLN:CD	0.45	2.75	3	1
1:A:216:LYS:CB	1:A:216:LYS:NZ	0.45	2.79	11	2
1:A:37:GLN:N	1:A:37:GLN:CD	0.45	2.75	8	2
1:A:186:ASP:O	1:A:190:VAL:HG12	0.45	2.11	5	1
1:A:53:GLU:N	1:A:53:GLU:CD	0.45	2.74	8	1
1:A:171:HIS:NE2	1:A:197:VAL:N	0.45	2.64	12	1
1:A:170:SER:O	1:A:198:ARG:CZ	0.45	2.65	8	2
1:A:53:GLU:CD	1:A:78:THR:H	0.45	2.20	11	1
1:A:132:HIS:CD2	1:A:209:LEU:HD21	0.45	2.47	13	1
2:B:30:GLU:N	2:B:30:GLU:OE2	0.45	2.49	13	1
1:A:138:MET:C	1:A:140:LYS:N	0.45	2.74	2	5
1:A:170:SER:O	1:A:198:ARG:CD	0.45	2.65	3	3
2:B:15:TYR:CG	2:B:53:ASP:OD1	0.45	2.69	8	1
1:A:162:HIS:C	1:A:162:HIS:ND1	0.45	2.75	12	1
1:A:211:VAL:HG12	1:A:212:LYS:N	0.45	2.27	15	1
2:B:27:ASP:CG	2:B:28:TYR:H	0.45	2.20	2	7
1:A:23:HIS:CB	1:A:202:MET:HE2	0.45	2.42	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:242:VAL:HG22	1:A:242:VAL:OXT	0.45	2.11	3	1
1:A:44:ILE:CG2	1:A:45:CYS:N	0.45	2.79	4	1
1:A:206:SER:O	1:A:207:SER:C	0.45	2.59	5	4
2:B:22:ARG:HH21	2:B:69:ASN:HD21	0.45	1.55	5	1
1:A:238:LEU:N	1:A:238:LEU:HD12	0.45	2.25	7	1
1:A:89:ARG:NH2	1:A:91:ASN:OD1	0.45	2.50	8	1
1:A:167:SER:C	1:A:169:ILE:N	0.44	2.74	15	3
2:B:33:SER:C	2:B:35:CYS:H	0.44	2.21	2	10
1:A:44:ILE:HG22	1:A:45:CYS:N	0.44	2.26	4	1
1:A:188:LYS:C	1:A:189:CYS:SG	0.44	2.99	6	1
1:A:168:ASN:N	1:A:168:ASN:OD1	0.44	2.50	9	1
2:B:34:LEU:N	2:B:34:LEU:HD12	0.44	2.27	10	2
1:A:29:ILE:HD12	1:A:198:ARG:NH2	0.44	2.26	11	1
1:A:162:HIS:ND1	1:A:162:HIS:C	0.44	2.75	1	1
2:B:42:PHE:CD1	2:B:42:PHE:O	0.44	2.71	4	1
1:A:190:VAL:HG22	1:A:190:VAL:O	0.44	2.12	6	1
1:A:21:LYS:O	1:A:22:HIS:ND1	0.44	2.50	9	1
1:A:90:MET:CE	1:A:92:PHE:CZ	0.44	3.01	13	1
1:A:100:ILE:O	1:A:100:ILE:CG2	0.44	2.66	13	1
1:A:186:ASP:OD1	1:A:186:ASP:N	0.44	2.50	13	4
1:A:29:ILE:HD13	1:A:171:HIS:NE2	0.44	2.27	10	1
1:A:196:SER:OG	1:A:198:ARG:CZ	0.44	2.66	11	1
1:A:172:LYS:C	1:A:198:ARG:HH12	0.44	2.20	12	1
1:A:172:LYS:CA	1:A:198:ARG:HH12	0.44	2.26	12	1
1:A:168:ASN:OD1	1:A:168:ASN:N	0.44	2.51	2	1
1:A:110:ASN:N	1:A:110:ASN:OD1	0.44	2.50	5	1
1:A:119:VAL:CG1	1:A:123:GLN:CD	0.44	2.91	7	1
1:A:165:LEU:N	1:A:165:LEU:HD22	0.44	2.26	8	1
1:A:215:PHE:CZ	2:B:14:SER:OG	0.44	2.71	14	1
1:A:80:TYR:CZ	1:A:82:SER:OG	0.44	2.65	15	1
2:B:27:ASP:OD2	2:B:29:TYR:CZ	0.44	2.71	15	1
1:A:30:ILE:H	1:A:115:ARG:HH21	0.44	1.56	2	1
1:A:34:LYS:CG	1:A:38:THR:OG1	0.44	2.65	7	1
1:A:21:LYS:NZ	1:A:129:ALA:O	0.44	2.51	15	2
1:A:169:ILE:C	1:A:169:ILE:CD1	0.44	2.90	14	1
1:A:82:SER:OG	1:A:89:ARG:NE	0.44	2.50	5	1
1:A:27:ASP:CG	1:A:171:HIS:NE2	0.44	2.76	6	2
2:B:22:ARG:CG	2:B:22:ARG:NH1	0.44	2.81	7	1
1:A:83:ILE:HD12	1:A:103:ILE:HD11	0.44	1.90	12	1
2:B:27:ASP:CG	2:B:28:TYR:N	0.44	2.75	2	8
1:A:130:ILE:H	1:A:130:ILE:CD1	0.44	2.25	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:SER:OG	2:B:51:CYS:O	0.44	2.36	9	1
1:A:27:ASP:OD1	1:A:29:ILE:CD1	0.44	2.66	10	1
2:B:43:GLN:CD	2:B:44:THR:H	0.44	2.21	11	1
1:A:141:ASP:OD2	2:B:18:ARG:CZ	0.44	2.66	14	1
2:B:29:TYR:CD2	2:B:30:GLU:N	0.44	2.85	7	3
1:A:212:LYS:NZ	1:A:226:ALA:CB	0.44	2.81	11	1
1:A:160:LYS:C	1:A:162:HIS:H	0.44	2.21	1	4
1:A:198:ARG:NH1	1:A:198:ARG:CG	0.44	2.80	7	3
1:A:125:LYS:NZ	1:A:127:SER:OG	0.44	2.42	7	1
2:B:48:ALA:O	2:B:49:GLN:NE2	0.44	2.51	7	1
2:B:34:LEU:CD1	2:B:34:LEU:H	0.44	2.25	11	2
2:B:22:ARG:O	2:B:23:ASN:C	0.43	2.61	9	3
1:A:43:LYS:NZ	1:A:154:GLU:O	0.43	2.45	12	1
1:A:176:TYR:O	1:A:176:TYR:CD2	0.43	2.70	6	2
1:A:53:GLU:CD	2:B:24:PHE:CZ	0.43	2.96	4	1
2:B:11:CYS:O	2:B:13:PHE:CZ	0.43	2.71	7	1
1:A:218:VAL:C	1:A:220:GLY:N	0.43	2.76	15	1
1:A:185:VAL:O	1:A:185:VAL:CG2	0.43	2.67	11	4
1:A:187:THR:C	1:A:189:CYS:H	0.43	2.20	6	1
1:A:88:LEU:CD2	1:A:88:LEU:C	0.43	2.92	9	1
1:A:160:LYS:NZ	1:A:240:ALA:H	0.43	2.08	10	1
1:A:187:THR:O	1:A:188:LYS:C	0.43	2.61	8	7
1:A:53:GLU:CD	1:A:54:SER:H	0.43	2.21	3	2
1:A:206:SER:H	1:A:210:GLU:CD	0.43	2.21	14	2
1:A:24:MET:SD	1:A:24:MET:N	0.43	2.91	8	1
1:A:88:LEU:N	1:A:88:LEU:HD13	0.43	2.29	9	1
1:A:193:LEU:HD12	1:A:195:PHE:CE2	0.43	2.48	11	1
1:A:113:ASN:HD22	1:A:114:ALA:N	0.43	2.09	3	1
1:A:234:ASP:C	1:A:236:THR:N	0.43	2.77	10	4
1:A:19:GLU:CD	1:A:19:GLU:H	0.43	2.21	4	1
1:A:12:SER:CB	1:A:125:LYS:O	0.43	2.67	7	2
1:A:151:SER:OG	1:A:152:GLU:N	0.43	2.51	9	1
1:A:147:ASP:OD1	1:A:147:ASP:C	0.43	2.62	13	1
1:A:99:GLN:CD	1:A:101:LYS:HZ3	0.43	2.21	14	1
1:A:180:ILE:HD12	1:A:180:ILE:O	0.43	2.13	15	1
1:A:180:ILE:O	1:A:180:ILE:HD13	0.43	2.14	5	1
1:A:83:ILE:C	1:A:83:ILE:CD1	0.43	2.91	7	2
1:A:44:ILE:O	1:A:45:CYS:C	0.43	2.62	13	1
1:A:97:CYS:O	1:A:98:PRO:C	0.43	2.62	11	8
1:A:233:ILE:C	1:A:233:ILE:CD1	0.43	2.91	2	1
1:A:183:THR:O	2:B:13:PHE:CE1	0.43	2.72	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:GLU:O	1:A:153:GLU:CD	0.43	2.61	6	1
1:A:135:ALA:O	1:A:138:MET:N	0.43	2.52	14	1
1:A:138:MET:SD	1:A:138:MET:N	0.43	2.91	6	1
1:A:37:GLN:N	1:A:37:GLN:NE2	0.43	2.66	8	1
1:A:27:ASP:CB	1:A:169:ILE:HD11	0.43	2.43	9	1
1:A:169:ILE:CG2	1:A:202:MET:HE1	0.43	2.43	13	1
1:A:143:GLU:CD	2:B:18:ARG:NE	0.43	2.76	15	1
1:A:143:GLU:CG	2:B:18:ARG:NE	0.43	2.82	15	1
1:A:235:SER:O	1:A:238:LEU:CD2	0.43	2.66	15	1
2:B:30:GLU:O	2:B:31:THR:O	0.43	2.37	14	12
2:B:19:LYS:NZ	2:B:58:TRP:CG	0.43	2.75	3	1
1:A:53:GLU:OE1	2:B:24:PHE:CE2	0.43	2.72	5	1
1:A:192:ASN:OD1	1:A:217:TYR:O	0.43	2.36	14	1
2:B:23:ASN:OD1	2:B:23:ASN:N	0.43	2.50	14	1
1:A:241:CYS:O	1:A:242:VAL:O	0.43	2.37	3	3
1:A:120:SER:O	1:A:121:PRO:O	0.43	2.37	8	1
1:A:132:HIS:CD2	1:A:132:HIS:C	0.42	2.96	2	1
1:A:45:CYS:H	1:A:105:GLU:CD	0.42	2.21	11	2
1:A:46:GLN:OE1	1:A:155:LYS:O	0.42	2.37	3	2
1:A:104:SER:HG	1:A:239:LYS:C	0.42	2.22	4	1
1:A:174:VAL:O	1:A:175:SER:O	0.42	2.37	4	1
1:A:206:SER:O	1:A:209:LEU:N	0.42	2.52	7	1
1:A:201:ASP:CG	1:A:204:LYS:H	0.42	2.22	13	1
1:A:92:PHE:CD2	1:A:94:PHE:CD1	0.42	3.08	5	1
1:A:111:THR:HG22	1:A:112:VAL:N	0.42	2.29	10	1
1:A:120:SER:O	1:A:123:GLN:OE1	0.42	2.36	13	2
1:A:237:LYS:N	1:A:237:LYS:CD	0.42	2.82	15	1
1:A:159:ILE:C	1:A:159:ILE:CD1	0.42	2.93	1	1
1:A:213:ASP:OD1	1:A:213:ASP:N	0.42	2.53	1	1
1:A:46:GLN:NE2	1:A:156:ASP:O	0.42	2.52	3	1
2:B:35:CYS:C	2:B:37:GLN:H	0.42	2.23	7	3
2:B:60:GLN:CD	2:B:60:GLN:N	0.42	2.77	9	1
1:A:80:TYR:CE2	1:A:92:PHE:O	0.42	2.72	12	1
2:B:41:VAL:HG12	2:B:51:CYS:SG	0.42	2.54	12	1
1:A:83:ILE:O	1:A:83:ILE:HG23	0.42	2.14	13	1
1:A:81:TYR:CD1	1:A:92:PHE:CE1	0.42	3.06	5	1
2:B:22:ARG:NH1	2:B:65:ASP:CG	0.42	2.77	5	1
1:A:202:MET:HE3	1:A:202:MET:N	0.42	2.28	7	1
1:A:151:SER:O	1:A:153:GLU:OE1	0.42	2.38	13	1
1:A:218:VAL:O	1:A:220:GLY:N	0.42	2.52	15	1
1:A:118:SER:OG	1:A:202:MET:SD	0.42	2.76	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:VAL:O	1:A:202:MET:HE1	0.42	2.13	1	1
1:A:22:HIS:CE1	1:A:132:HIS:CD2	0.42	3.07	3	1
1:A:197:VAL:HG12	1:A:198:ARG:N	0.42	2.29	5	3
1:A:227:THR:HG22	1:A:228:ASP:N	0.42	2.30	5	2
1:A:232:LEU:O	1:A:232:LEU:HD13	0.42	2.15	9	2
1:A:218:VAL:O	1:A:219:ASP:CG	0.42	2.62	10	1
1:A:191:LYS:CD	1:A:191:LYS:C	0.42	2.92	14	1
1:A:172:LYS:CG	1:A:173:LYS:N	0.42	2.82	5	1
1:A:173:LYS:CB	1:A:173:LYS:NZ	0.42	2.83	13	1
1:A:130:ILE:HD11	1:A:134:GLU:OE2	0.42	2.15	3	1
1:A:178:ASP:OD1	1:A:178:ASP:N	0.42	2.52	4	2
1:A:182:SER:CB	2:B:51:CYS:H	0.42	2.26	10	2
1:A:80:TYR:O	1:A:80:TYR:CG	0.42	2.73	13	1
1:A:122:GLY:N	1:A:123:GLN:OE1	0.42	2.53	13	1
1:A:91:ASN:N	1:A:91:ASN:ND2	0.42	2.64	3	1
1:A:241:CYS:O	1:A:241:CYS:SG	0.42	2.77	8	3
2:B:42:PHE:C	2:B:42:PHE:CD1	0.42	2.98	3	1
1:A:172:LYS:N	1:A:198:ARG:NH1	0.42	2.66	12	1
1:A:169:ILE:CD1	1:A:169:ILE:C	0.42	2.92	13	1
1:A:11:SER:OG	1:A:127:SER:O	0.42	2.38	14	1
1:A:233:ILE:HD12	1:A:233:ILE:O	0.42	2.15	2	1
1:A:80:TYR:C	1:A:81:TYR:CD1	0.42	2.98	7	1
1:A:170:SER:CB	1:A:172:LYS:NZ	0.42	2.83	8	1
1:A:171:HIS:CD2	1:A:198:ARG:HH21	0.42	2.32	11	1
1:A:24:MET:CE	1:A:135:ALA:HB1	0.42	2.44	9	2
1:A:141:ASP:O	1:A:143:GLU:OE1	0.42	2.38	14	1
1:A:148:ILE:HD12	1:A:148:ILE:C	0.41	2.40	4	1
1:A:115:ARG:C	1:A:116:LEU:HD22	0.41	2.40	6	1
1:A:230:THR:HG23	1:A:231:SER:N	0.41	2.30	7	2
1:A:206:SER:C	1:A:208:GLU:N	0.41	2.77	8	1
1:A:80:TYR:OH	1:A:91:ASN:ND2	0.41	2.53	10	1
1:A:231:SER:O	1:A:232:LEU:C	0.41	2.63	9	6
1:A:51:ILE:HG22	1:A:52:THR:N	0.41	2.30	5	1
1:A:184:ILE:O	1:A:184:ILE:CG2	0.41	2.68	7	1
1:A:131:THR:CG2	1:A:132:HIS:N	0.41	2.82	8	1
1:A:29:ILE:N	1:A:29:ILE:CD1	0.41	2.83	10	1
1:A:27:ASP:CG	1:A:117:SER:OG	0.41	2.63	11	1
1:A:81:TYR:CE2	1:A:92:PHE:CD1	0.41	3.09	11	1
1:A:167:SER:OG	1:A:202:MET:SD	0.41	2.74	13	1
1:A:238:LEU:CD2	1:A:238:LEU:H	0.41	2.28	15	1
1:A:160:LYS:C	1:A:162:HIS:N	0.41	2.76	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:ASP:OD1	1:A:228:ASP:N	0.41	2.53	3	1
1:A:234:ASP:O	1:A:234:ASP:OD1	0.41	2.39	6	2
1:A:162:HIS:O	1:A:163:PRO:C	0.41	2.64	13	4
1:A:81:TYR:CE2	1:A:92:PHE:CB	0.41	3.04	10	1
1:A:147:ASP:OD2	2:B:49:GLN:NE2	0.41	2.52	12	1
1:A:46:GLN:OE1	1:A:153:GLU:O	0.41	2.39	2	1
1:A:27:ASP:OD2	1:A:171:HIS:NE2	0.41	2.54	10	1
1:A:29:ILE:CD1	1:A:171:HIS:HE2	0.41	2.29	10	1
1:A:133:GLU:N	1:A:133:GLU:OE1	0.41	2.53	14	1
1:A:19:GLU:CD	1:A:19:GLU:N	0.41	2.78	8	1
1:A:177:GLU:OE1	1:A:212:LYS:O	0.41	2.39	8	1
1:A:43:LYS:C	1:A:46:GLN:HE22	0.41	2.22	4	1
1:A:175:SER:OG	1:A:210:GLU:O	0.41	2.38	4	1
1:A:241:CYS:O	1:A:242:VAL:C	0.41	2.63	8	2
2:B:56:GLU:C	2:B:60:GLN:HE22	0.41	2.23	5	1
1:A:123:GLN:OE1	1:A:125:LYS:O	0.41	2.39	6	1
1:A:143:GLU:CD	1:A:143:GLU:C	0.41	2.89	11	4
2:B:43:GLN:OE1	2:B:48:ALA:O	0.41	2.39	11	1
1:A:211:VAL:HG22	1:A:212:LYS:N	0.41	2.31	12	1
1:A:198:ARG:NH2	1:A:205:GLU:OE2	0.41	2.54	13	1
1:A:141:ASP:O	1:A:143:GLU:OE2	0.41	2.39	15	1
1:A:26:ILE:CD1	1:A:27:ASP:N	0.41	2.83	4	1
1:A:120:SER:O	1:A:121:PRO:C	0.41	2.64	12	3
1:A:24:MET:HE1	1:A:209:LEU:HB3	0.41	1.92	9	1
1:A:17:GLU:CD	1:A:17:GLU:O	0.41	2.63	3	1
1:A:52:THR:O	1:A:53:GLU:O	0.41	2.38	8	2
1:A:95:THR:HG21	2:B:18:ARG:NE	0.41	2.31	3	1
2:B:67:GLU:CD	2:B:67:GLU:C	0.41	2.88	7	2
1:A:132:HIS:CE1	1:A:209:LEU:HD21	0.41	2.50	8	1
1:A:192:ASN:CG	1:A:217:TYR:O	0.41	2.64	4	3
2:B:15:TYR:CG	2:B:53:ASP:CG	0.41	2.99	2	1
1:A:23:HIS:HB2	1:A:202:MET:HE2	0.41	1.92	3	1
1:A:143:GLU:C	1:A:143:GLU:CD	0.41	2.89	5	1
1:A:189:CYS:O	1:A:189:CYS:SG	0.41	2.78	5	1
1:A:41:ASN:N	1:A:41:ASN:HD22	0.41	2.12	6	1
1:A:52:THR:C	1:A:53:GLU:O	0.41	2.62	6	1
1:A:35:GLN:C	1:A:37:GLN:H	0.41	2.24	7	2
1:A:121:PRO:CD	1:A:202:MET:SD	0.41	3.09	7	1
1:A:35:GLN:O	1:A:37:GLN:N	0.41	2.54	8	1
1:A:29:ILE:CD1	1:A:171:HIS:NE2	0.41	2.83	10	1
1:A:41:ASN:ND2	1:A:41:ASN:C	0.41	2.78	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:23:ASN:O	2:B:23:ASN:OD1	0.41	2.39	11	1
1:A:181:GLY:O	2:B:14:SER:OG	0.41	2.39	12	1
1:A:127:SER:OG	1:A:127:SER:O	0.41	2.37	14	1
1:A:142:CYS:O	1:A:143:GLU:OE2	0.41	2.39	14	1
1:A:141:ASP:O	1:A:143:GLU:CD	0.41	2.64	15	1
1:A:104:SER:C	1:A:105:GLU:CD	0.41	2.89	10	1
2:B:27:ASP:OD1	2:B:43:GLN:CD	0.41	2.64	13	1
1:A:20:ASN:N	1:A:20:ASN:ND2	0.41	2.65	14	1
1:A:23:HIS:NE2	1:A:121:PRO:CG	0.41	2.84	15	1
1:A:41:ASN:ND2	1:A:86:GLY:O	0.40	2.55	1	1
1:A:138:MET:O	1:A:140:LYS:N	0.40	2.54	13	2
1:A:104:SER:OG	1:A:239:LYS:O	0.40	2.40	3	2
1:A:141:ASP:O	1:A:142:CYS:C	0.40	2.64	7	2
1:A:29:ILE:HD11	1:A:171:HIS:CE1	0.40	2.51	8	1
1:A:194:GLU:OE1	1:A:232:LEU:HD21	0.40	2.16	9	1
2:B:56:GLU:O	2:B:60:GLN:OE1	0.40	2.39	9	1
1:A:23:HIS:O	1:A:24:MET:O	0.40	2.39	14	1
1:A:27:ASP:OD2	1:A:198:ARG:O	0.40	2.39	5	1
1:A:115:ARG:HH21	1:A:238:LEU:CD2	0.40	2.30	5	1
2:B:33:SER:O	2:B:35:CYS:N	0.40	2.54	11	1
1:A:141:ASP:O	1:A:141:ASP:OD1	0.40	2.39	12	1
1:A:102:SER:OG	1:A:117:SER:O	0.40	2.38	13	1
1:A:104:SER:C	1:A:105:GLU:OE2	0.40	2.65	2	2
1:A:108:ASP:OD1	1:A:108:ASP:N	0.40	2.55	2	1
1:A:177:GLU:OE2	1:A:178:ASP:O	0.40	2.39	2	1
1:A:143:GLU:OE2	1:A:144:VAL:C	0.40	2.64	3	1
1:A:41:ASN:O	1:A:41:ASN:OD1	0.40	2.40	4	1
1:A:180:ILE:HD12	1:A:213:ASP:OD2	0.40	2.17	5	1
1:A:80:TYR:CE1	1:A:82:SER:OG	0.40	2.74	6	1
1:A:36:ASP:C	1:A:37:GLN:NE2	0.40	2.79	8	1
1:A:194:GLU:N	1:A:194:GLU:OE1	0.40	2.54	12	1
1:A:43:LYS:O	1:A:46:GLN:OE1	0.40	2.39	4	1
1:A:153:GLU:O	1:A:153:GLU:OE1	0.40	2.40	6	1
1:A:195:PHE:CD1	1:A:195:PHE:C	0.40	2.99	6	1
1:A:44:ILE:O	1:A:157:SER:OG	0.40	2.40	9	1
1:A:46:GLN:O	1:A:46:GLN:CD	0.40	2.65	9	1
1:A:143:GLU:OE1	2:B:17:ALA:N	0.40	2.51	9	1
1:A:156:ASP:CG	1:A:157:SER:H	0.40	2.25	10	1
1:A:218:VAL:O	1:A:219:ASP:OD1	0.40	2.40	10	1
1:A:146:ILE:C	1:A:147:ASP:CG	0.40	2.90	12	1
2:B:49:GLN:CD	2:B:49:GLN:C	0.40	2.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:CYS:O	1:A:98:PRO:O	0.40	2.39	13	1
1:A:152:GLU:O	1:A:154:GLU:OE2	0.40	2.40	14	1
1:A:50:GLU:CD	1:A:50:GLU:C	0.40	2.90	1	1
1:A:50:GLU:O	1:A:50:GLU:OE2	0.40	2.40	2	1
2:B:48:ALA:O	2:B:49:GLN:OE1	0.40	2.40	2	1
1:A:26:ILE:HD13	1:A:27:ASP:H	0.40	1.75	4	1
1:A:21:LYS:H	1:A:21:LYS:HD3	0.40	1.75	5	1
1:A:90:MET:SD	1:A:148:ILE:HD12	0.40	2.57	6	1
1:A:147:ASP:CG	1:A:184:ILE:CG2	0.40	2.94	7	1
1:A:43:LYS:O	1:A:46:GLN:NE2	0.40	2.55	8	1
1:A:222:ALA:O	1:A:223:SER:OG	0.40	2.40	9	1
1:A:35:GLN:NE2	1:A:36:ASP:N	0.40	2.70	10	1
1:A:46:GLN:CD	1:A:46:GLN:C	0.40	2.90	10	1
2:B:28:TYR:OH	2:B:67:GLU:OE2	0.40	2.40	11	1
1:A:152:GLU:O	1:A:154:GLU:OE1	0.40	2.40	14	1
1:A:183:THR:O	1:A:183:THR:OG1	0.40	2.40	15	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/242 (88%)	168±4 (79±2%)	34±3 (16±1%)	10±2 (5±1%)	3	25
2	B	59/69 (86%)	41±2 (70±3%)	14±3 (23±4%)	4±1 (7±2%)	2	16
All	All	4065/4665 (87%)	3142 (77%)	711 (17%)	212 (5%)	3	23

All 49 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	31	THR	15
2	B	48	ALA	15
1	A	163	PRO	13
1	A	207	SER	11
1	A	39	PRO	10

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Mol	Chain	Res	Type	Models (Total)
1	A	93	GLY	10
1	A	53	GLU	10
1	A	188	LYS	9
1	A	98	PRO	9
1	A	228	ASP	8
2	B	10	ALA	8
1	A	121	PRO	6
1	A	8	SER	6
1	A	18	GLU	6
2	B	23	ASN	6
1	A	190	VAL	5
2	B	38	PRO	5
1	A	43	LYS	5
1	A	19	GLU	4
2	B	25	VAL	4
1	A	77	PRO	3
1	A	172	LYS	3
1	A	175	SER	3
1	A	153	GLU	2
1	A	174	VAL	2
1	A	232	LEU	2
2	B	39	ALA	2
2	B	44	THR	2
1	A	128	PRO	2
1	A	24	MET	2
1	A	219	ASP	2
1	A	54	SER	2
1	A	48	VAL	2
1	A	156	ASP	2
1	A	152	GLU	2
1	A	37	GLN	1
1	A	205	GLU	1
1	A	155	LYS	1
1	A	193	LEU	1
2	B	37	GLN	1
1	A	199	ILE	1
2	B	21	PRO	1
1	A	123	GLN	1
2	B	47	SER	1
1	A	235	SER	1
1	A	45	CYS	1
1	A	171	HIS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	32	SER	1
1	A	30	ILE	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	191/219 (87%)	176±4 (92±2%)	15±4 (8±2%)	14	61
2	B	53/60 (88%)	51±1 (96±2%)	2±1 (4±2%)	27	77
All	All	3660/4185 (87%)	3401 (93%)	259 (7%)	15	64

All 111 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	80	TYR	8
1	A	232	LEU	8
1	A	24	MET	6
1	A	130	ILE	6
2	B	18	ARG	6
1	A	212	LYS	5
2	B	67	GLU	5
1	A	171	HIS	5
1	A	94	PHE	5
1	A	153	GLU	5
1	A	202	MET	5
1	A	41	ASN	4
1	A	44	ILE	4
1	A	52	THR	4
1	A	160	LYS	4
1	A	238	LEU	4
1	A	81	TYR	4
1	A	116	LEU	4
1	A	233	ILE	4
2	B	15	TYR	4
2	B	68	LEU	4
1	A	120	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	183	THR	4
1	A	236	THR	4
1	A	242	VAL	4
2	B	41	VAL	4
1	A	96	LYS	4
1	A	103	ILE	3
1	A	172	LYS	3
1	A	185	VAL	3
1	A	193	LEU	3
1	A	195	PHE	3
1	A	83	ILE	3
1	A	174	VAL	3
1	A	91	ASN	3
1	A	46	GLN	3
1	A	131	THR	3
1	A	139	ILE	3
1	A	113	ASN	3
1	A	54	SER	2
1	A	167	SER	2
1	A	106	SER	2
1	A	111	THR	2
1	A	148	ILE	2
1	A	177	GLU	2
1	A	90	MET	2
1	A	92	PHE	2
1	A	180	ILE	2
1	A	190	VAL	2
1	A	97	CYS	2
1	A	112	VAL	2
1	A	188	LYS	2
2	B	24	PHE	2
2	B	56	GLU	2
1	A	32	VAL	2
1	A	209	LEU	2
2	B	13	PHE	2
1	A	169	ILE	2
1	A	198	ARG	2
1	A	210	GLU	2
1	A	34	LYS	2
1	A	143	GLU	2
1	A	53	GLU	1
1	A	187	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	213	ASP	1
1	A	50	GLU	1
2	B	20	LEU	1
1	A	162	HIS	1
1	A	26	ILE	1
1	A	192	ASN	1
2	B	36	SER	1
1	A	184	ILE	1
2	B	69	ASN	1
1	A	123	GLN	1
1	A	15	CYS	1
1	A	16	THR	1
1	A	18	GLU	1
1	A	21	LYS	1
1	A	84	ILE	1
1	A	99	GLN	1
1	A	125	LYS	1
1	A	196	SER	1
1	A	199	ILE	1
1	A	211	VAL	1
2	B	51	CYS	1
1	A	23	HIS	1
1	A	146	ILE	1
1	A	159	ILE	1
1	A	204	LYS	1
1	A	237	LYS	1
1	A	88	LEU	1
1	A	208	GLU	1
2	B	12	CYS	1
1	A	35	GLN	1
1	A	216	LYS	1
1	A	241	CYS	1
1	A	100	ILE	1
1	A	101	LYS	1
1	A	173	LYS	1
1	A	20	ASN	1
1	A	30	ILE	1
1	A	43	LYS	1
1	A	133	GLU	1
1	A	191	LYS	1
1	A	224	LYS	1
1	A	29	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	37	GLN	1
1	A	48	VAL	1
1	A	179	ILE	1
1	A	217	TYR	1
2	B	19	LYS	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