



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:44 AM BST

PDB ID : 2Z2D
Title : Solution structure of human macrophage elastase (MMP-12) catalytic domain complexed with a gamma-keto butanoic acid inhibitor
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Deposited on : 2007-05-18

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

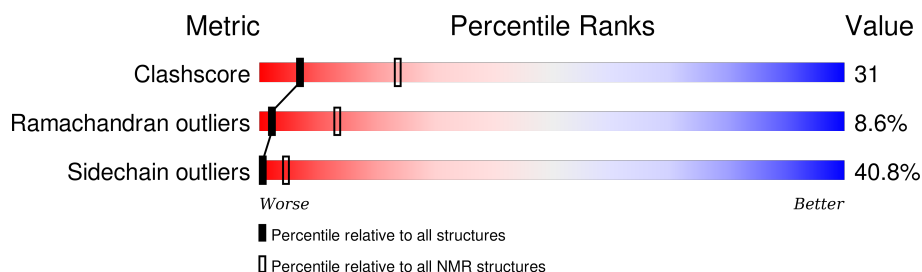
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	164	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:110-A:168, A:173-A:260 (147)	0.72	6

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2470 atoms, of which 1197 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	158	Total	C	H	N	O	S	0
			2412	794	1172	216	227	3	

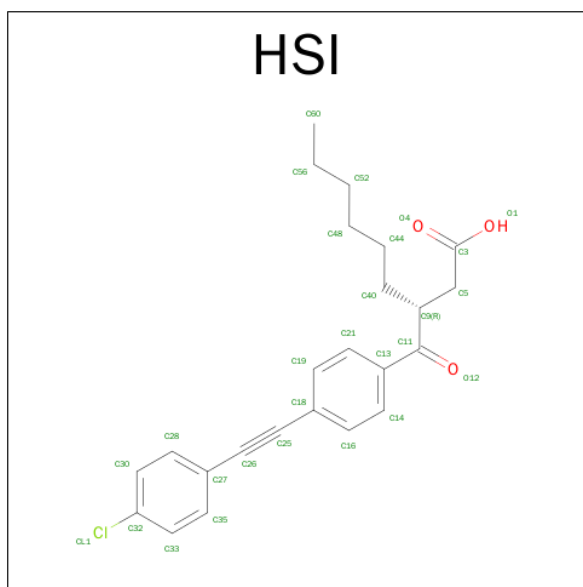
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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

Mol	Chain	Residues	Atoms	
3	A	3	Total	Ca
			3	3

- Molecule 4 is (3R)-3-{4-[(4-CHLOROPHENYL)ETHYNYL]BENZOYL}NONANOIC ACID (three-letter code: HSI) (formula: C₂₄H₂₅ClO₃).



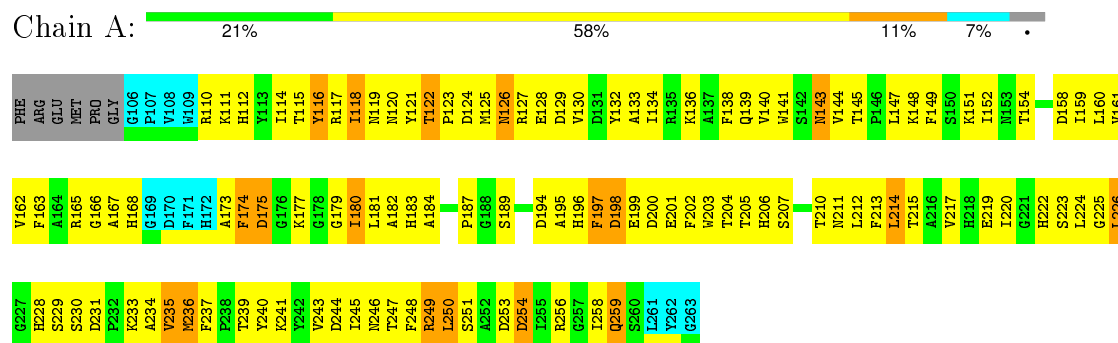
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	Cl	H	O
			53	24	1	25	3

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: Macrophage metalloelastase

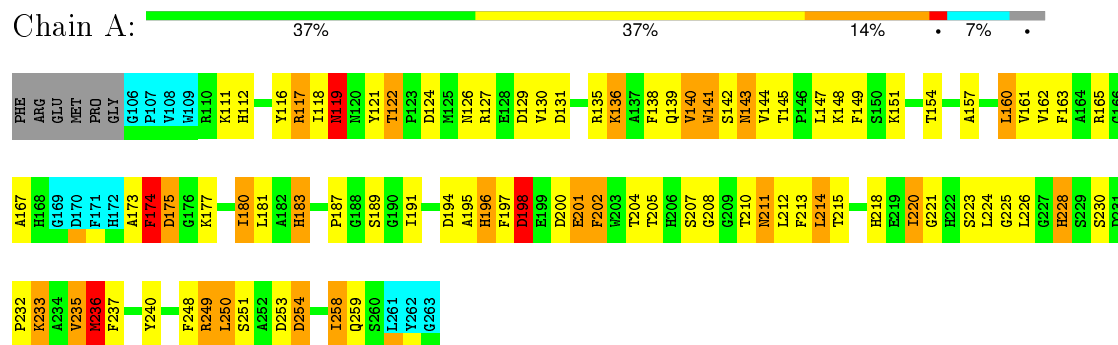


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

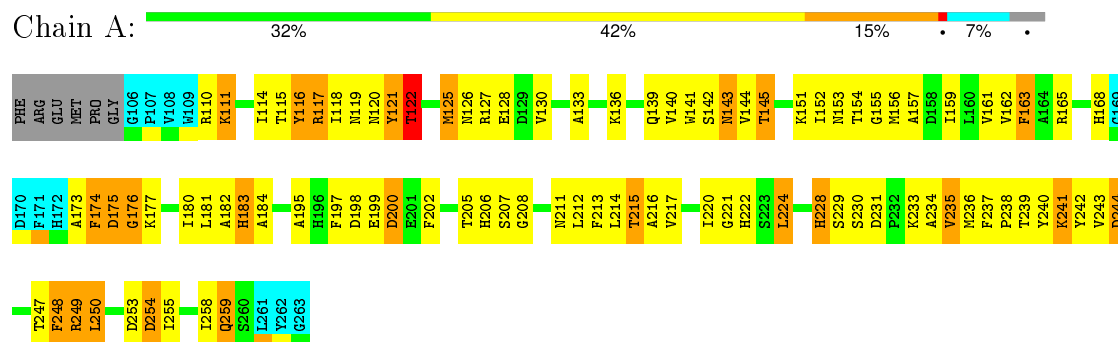
4.2.1 Score per residue for model 1

- Molecule 1: Macrophage metalloelastase



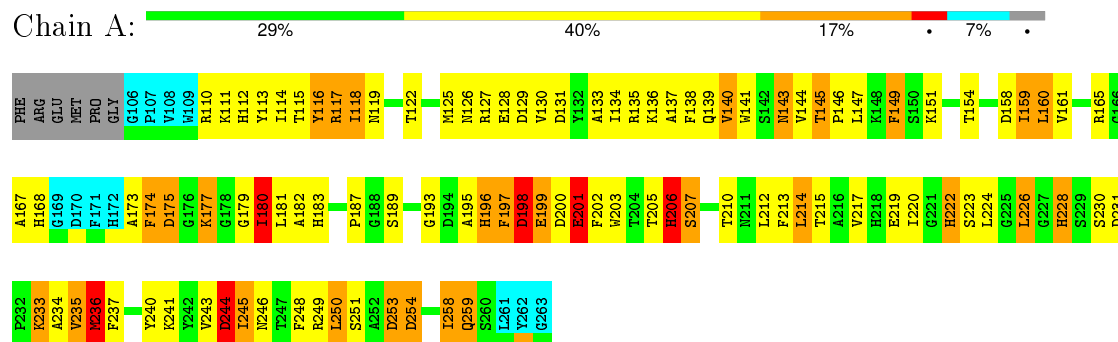
4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase



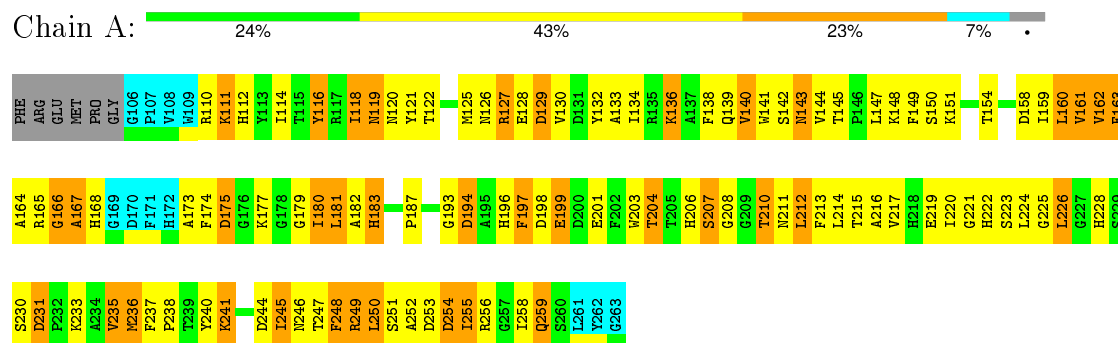
4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



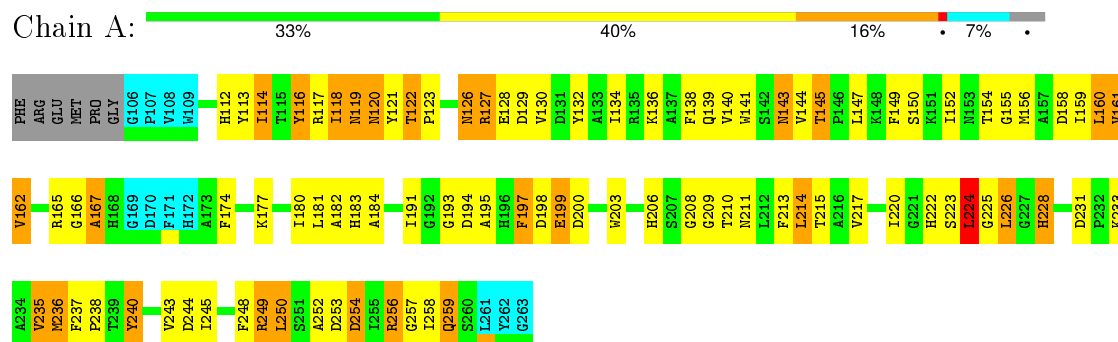
4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase



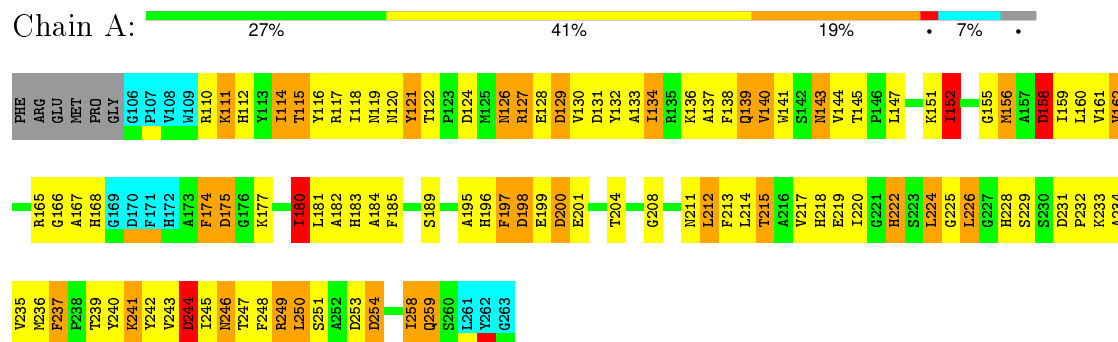
4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase



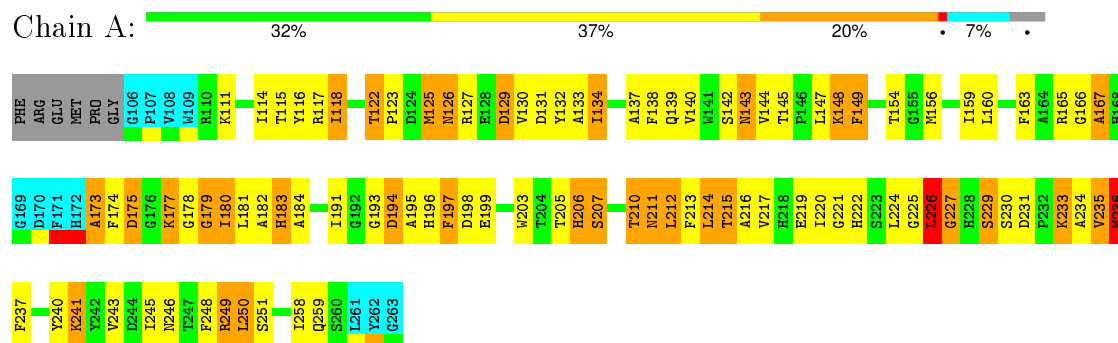
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Macrophage metalloelastase



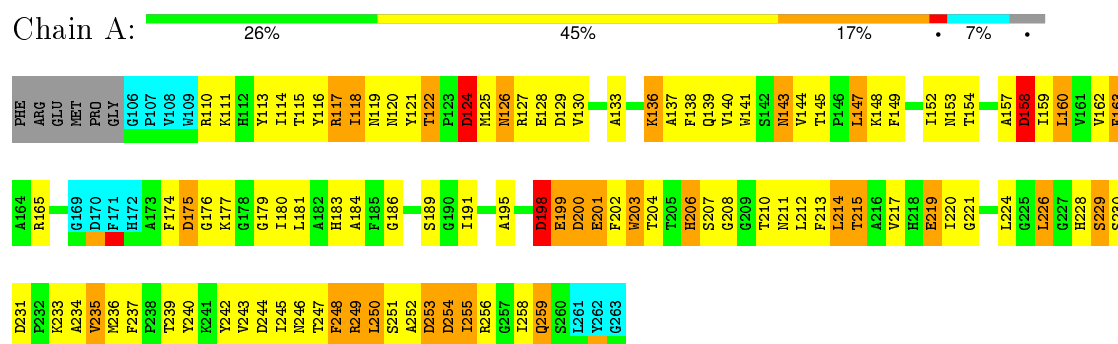
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



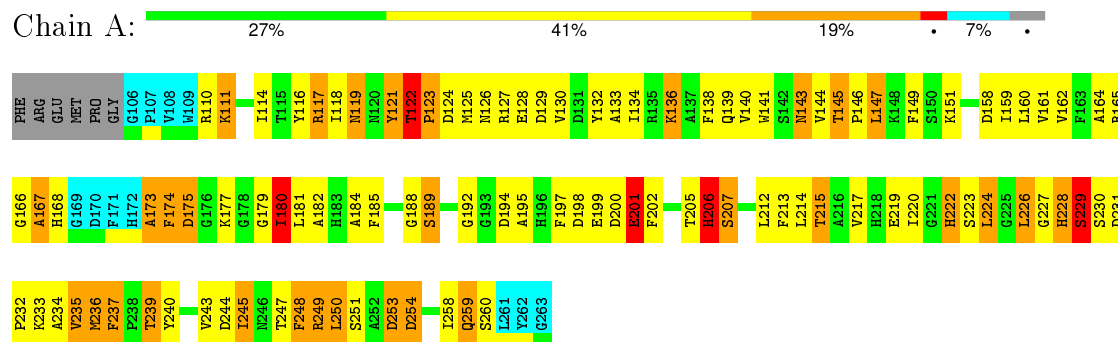
4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase



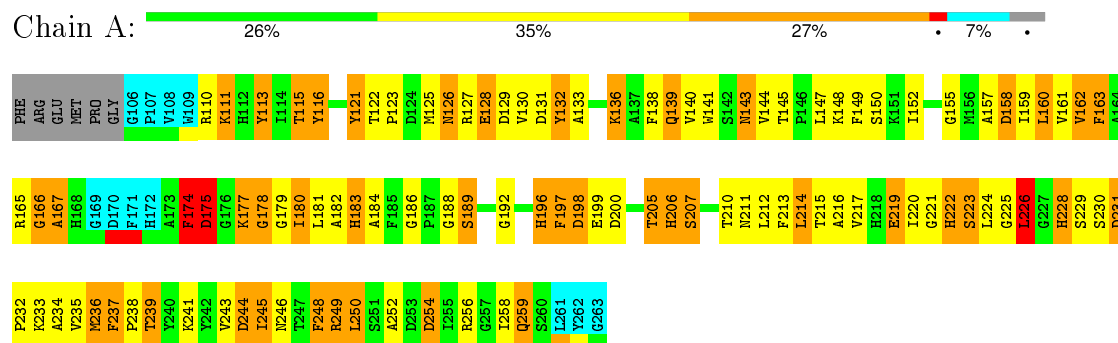
4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase



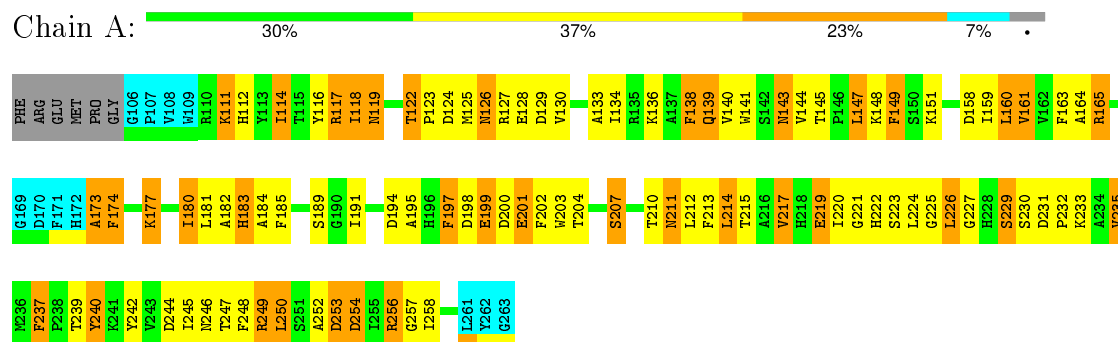
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



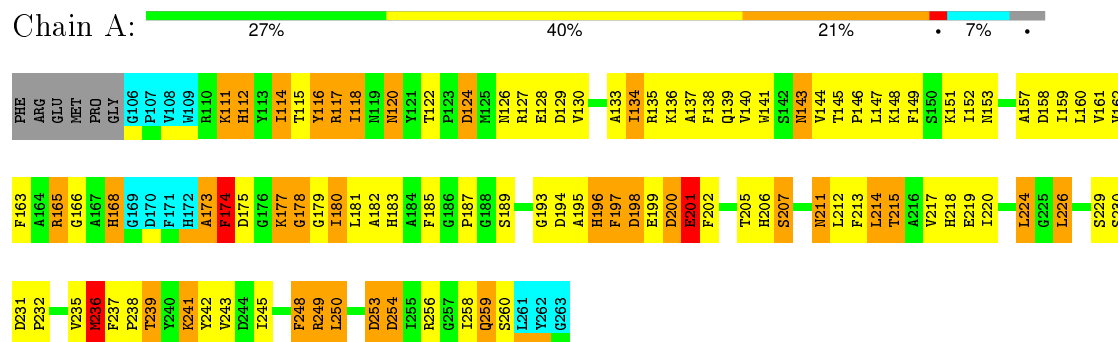
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



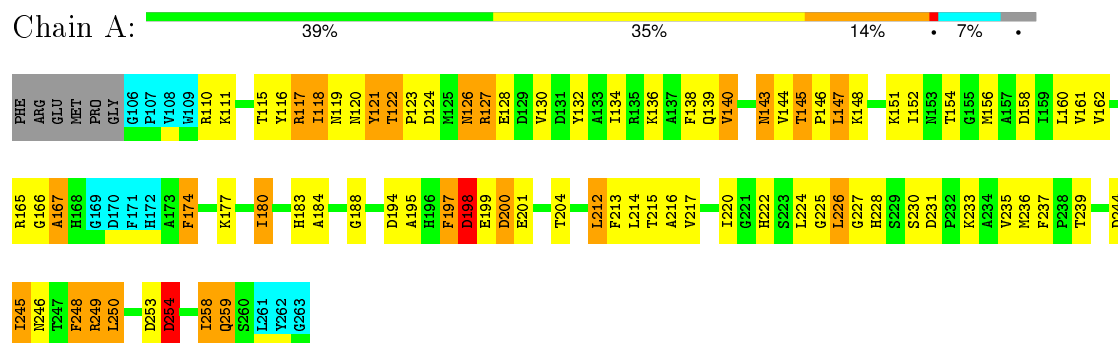
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



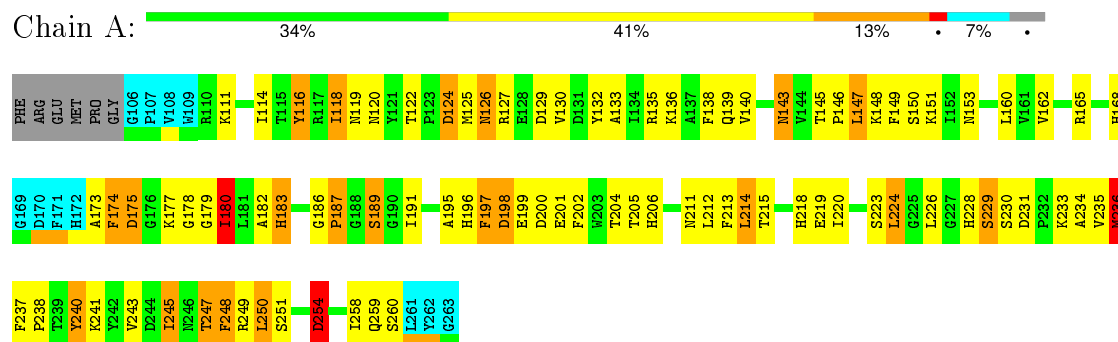
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



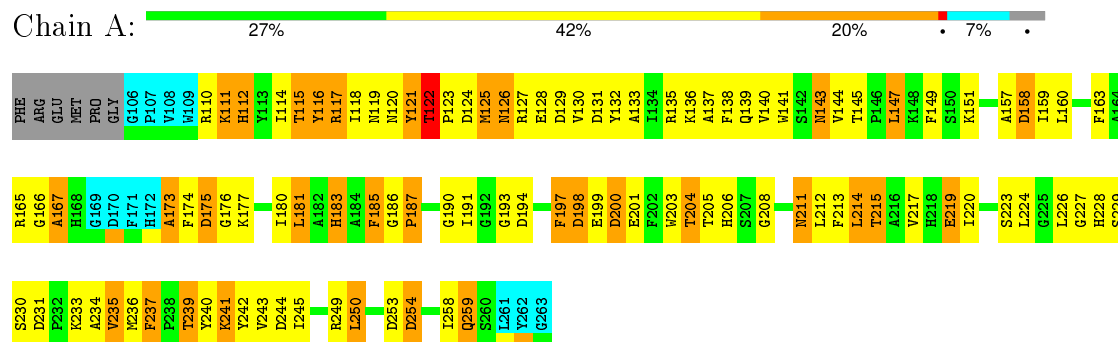
4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase



4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Distance geometry, simulated annealing, torsion angle dynamics*.

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Cyana	structure solution	2.1
Cyana	refinement	2.1

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HSI, CA

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	0.86±0.08	0±0/1184 (0.0±0.0%)	1.16±0.14	8±4/1605 (0.5±0.2%)
All	All	0.86	0/17760 (0.0%)	1.17	122/24075 (0.5%)

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	0.2±0.4
All	All	0	3

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	124	ASP	CB-CG-OD2	-13.16	106.45	118.30	15	6
1	A	244	ASP	CB-CG-OD2	-11.08	108.33	118.30	6	3
1	A	158	ASP	CB-CG-OD2	-10.57	108.79	118.30	8	8
1	A	231	ASP	CB-CG-OD2	-9.95	109.34	118.30	3	10
1	A	175	ASP	CB-CG-OD2	-9.77	109.50	118.30	3	6
1	A	175	ASP	CB-CG-OD1	-9.76	109.52	118.30	15	2
1	A	199	GLU	OE1-CD-OE2	9.41	134.59	123.30	3	9
1	A	254	ASP	CB-CG-OD2	-9.07	110.14	118.30	8	10
1	A	219	GLU	OE1-CD-OE2	8.50	133.50	123.30	8	3
1	A	198	ASP	CA-CB-CG	-8.49	94.71	113.40	13	1
1	A	128	GLU	OE1-CD-OE2	7.46	132.25	123.30	15	10
1	A	253	ASP	CB-CG-OD2	-7.40	111.64	118.30	15	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	200	ASP	CB-CG-OD2	-7.40	111.64	118.30	3	8
1	A	129	ASP	CB-CG-OD2	-7.35	111.69	118.30	8	8
1	A	244	ASP	OD1-CG-OD2	7.19	136.96	123.30	3	1
1	A	244	ASP	CB-CG-OD1	-6.95	112.04	118.30	3	1
1	A	131	ASP	CB-CG-OD2	-6.88	112.11	118.30	3	2
1	A	198	ASP	CB-CG-OD2	-6.82	112.16	118.30	6	4
1	A	198	ASP	CB-CG-OD1	6.82	124.44	118.30	7	3
1	A	158	ASP	CB-CG-OD1	-6.74	112.23	118.30	10	1
1	A	201	GLU	OE1-CD-OE2	6.44	131.03	123.30	8	4
1	A	158	ASP	OD1-CG-OD2	6.22	135.12	123.30	8	2
1	A	135	ARG	NE-CZ-NH2	-6.17	117.21	120.30	1	1
1	A	124	ASP	OD1-CG-OD2	6.03	134.75	123.30	15	1
1	A	135	ARG	NE-CZ-NH1	6.02	123.31	120.30	1	1
1	A	131	ASP	CB-CG-OD1	-5.85	113.03	118.30	6	1
1	A	141	TRP	CD1-NE1-CE2	5.81	114.23	109.00	1	1
1	A	231	ASP	OD1-CG-OD2	5.46	133.68	123.30	15	1
1	A	254	ASP	OD1-CG-OD2	5.21	133.20	123.30	15	1
1	A	256	ARG	NE-CZ-NH1	5.17	122.89	120.30	11	1
1	A	127	ARG	NE-CZ-NH1	5.17	122.88	120.30	13	1
1	A	200	ASP	CB-CG-OD1	-5.08	113.73	118.30	12	1
1	A	254	ASP	CB-CG-OD1	-5.05	113.76	118.30	9	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	198	ASP	Sidechain	3

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	1151	1098	1098	72±14
4	A	28	25	24	4±2
All	All	17760	16845	16830	1085

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:243:VAL:HG11	4:A:269:HSI:C33	0.92	1.93	6	2
1:A:181:LEU:HD21	1:A:215:THR:HG23	0.91	1.39	6	1
1:A:184:ALA:HB2	1:A:195:ALA:HB2	0.90	1.43	9	8
1:A:214:LEU:HD11	4:A:269:HSI:H19	0.88	1.41	15	4
1:A:213:PHE:O	1:A:217:VAL:HG23	0.88	1.69	8	10
1:A:116:TYR:CZ	1:A:159:ILE:HD13	0.82	2.10	6	1
1:A:116:TYR:CE2	1:A:159:ILE:HD13	0.82	2.09	6	1
1:A:159:ILE:HG23	1:A:193:GLY:O	0.81	1.75	7	3
1:A:235:VAL:O	4:A:269:HSI:H28	0.80	1.76	5	2
1:A:213:PHE:CE1	1:A:245:ILE:HG23	0.79	2.12	15	3
1:A:181:LEU:HD22	1:A:240:TYR:CE1	0.79	2.12	15	2
1:A:116:TYR:OH	1:A:118:ILE:HD12	0.79	1.77	12	1
1:A:161:VAL:HG13	1:A:197:PHE:CE1	0.79	2.12	3	5
1:A:213:PHE:CZ	1:A:245:ILE:HG23	0.77	2.15	15	2
1:A:159:ILE:HG22	1:A:193:GLY:HA3	0.76	1.58	12	1
1:A:144:VAL:HG11	1:A:255:ILE:HG21	0.76	1.58	8	2
1:A:126:ASN:O	1:A:130:VAL:HG23	0.75	1.81	2	14
1:A:224:LEU:HD12	1:A:225:GLY:N	0.75	1.97	7	5
1:A:145:THR:HG21	1:A:224:LEU:HD13	0.74	1.60	7	2
1:A:213:PHE:CD2	1:A:245:ILE:HG23	0.74	2.17	11	1
1:A:181:LEU:CD2	1:A:215:THR:HG23	0.73	2.12	6	1
1:A:137:ALA:HB1	1:A:220:ILE:HD11	0.73	1.58	15	3
1:A:140:VAL:CG1	1:A:250:LEU:HD11	0.73	2.14	8	1
1:A:129:ASP:HB3	1:A:205:THR:HG21	0.73	1.61	14	1
1:A:143:ASN:ND2	1:A:144:VAL:HG13	0.72	1.99	4	13
1:A:182:ALA:HB3	1:A:215:THR:HG21	0.72	1.61	2	1
1:A:211:ASN:CB	1:A:245:ILE:HD11	0.72	2.15	5	2
1:A:184:ALA:HB2	1:A:195:ALA:CB	0.71	2.14	9	5
1:A:136:LYS:O	1:A:140:VAL:HG23	0.70	1.86	14	3
1:A:220:ILE:O	1:A:224:LEU:HD23	0.70	1.86	6	1
1:A:141:TRP:CD2	1:A:224:LEU:HD11	0.70	2.21	15	2
1:A:125:MET:SD	1:A:130:VAL:HG22	0.70	2.27	8	3
1:A:140:VAL:HG13	1:A:250:LEU:HD21	0.70	1.62	2	1
1:A:213:PHE:CE2	1:A:245:ILE:HG23	0.69	2.22	11	1
1:A:214:LEU:O	1:A:214:LEU:HD12	0.69	1.88	3	1
1:A:229:SER:OG	1:A:234:ALA:HB2	0.69	1.86	15	4
1:A:198:ASP:CG	1:A:198:ASP:O	0.69	2.31	10	3
1:A:250:LEU:N	1:A:250:LEU:HD13	0.68	2.02	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ALA:CB	1:A:217:VAL:HG22	0.68	2.17	15	4
1:A:133:ALA:CB	1:A:212:LEU:HD21	0.68	2.17	2	1
1:A:181:LEU:HD23	1:A:215:THR:HG23	0.68	1.66	8	5
1:A:157:ALA:O	1:A:160:LEU:HD13	0.67	1.90	8	1
1:A:116:TYR:CE2	1:A:138:PHE:CE2	0.67	2.83	4	2
1:A:161:VAL:HG12	1:A:197:PHE:CE2	0.67	2.25	4	1
1:A:141:TRP:CZ3	1:A:258:ILE:HD13	0.67	2.25	10	4
1:A:211:ASN:HB2	1:A:245:ILE:HD11	0.67	1.67	7	2
1:A:245:ILE:HD12	1:A:245:ILE:H	0.67	1.49	6	1
1:A:115:THR:O	1:A:159:ILE:HD12	0.67	1.89	6	1
1:A:133:ALA:HB3	1:A:212:LEU:HD12	0.66	1.67	10	8
1:A:234:ALA:HB3	1:A:237:PHE:HB3	0.66	1.66	15	4
1:A:250:LEU:HD13	1:A:250:LEU:N	0.66	2.06	15	7
1:A:152:ILE:HD12	1:A:154:THR:HG22	0.66	1.67	5	1
1:A:118:ILE:HD11	1:A:134:ILE:CD1	0.66	2.20	6	1
1:A:140:VAL:O	1:A:144:VAL:HG22	0.66	1.90	12	13
1:A:141:TRP:O	1:A:145:THR:HG22	0.66	1.91	5	1
1:A:116:TYR:CE1	1:A:118:ILE:HD12	0.65	2.25	13	2
1:A:181:LEU:HD12	1:A:203:TRP:CH2	0.65	2.26	5	1
1:A:212:LEU:C	1:A:212:LEU:HD13	0.65	2.12	7	2
1:A:160:LEU:HD11	1:A:162:VAL:HG12	0.65	1.69	10	1
1:A:163:PHE:N	1:A:163:PHE:CD1	0.65	2.60	10	1
1:A:237:PHE:HE1	4:A:269:HSI:C26	0.65	2.04	10	2
1:A:115:THR:HB	1:A:157:ALA:HB1	0.65	1.68	10	1
1:A:130:VAL:HG13	1:A:212:LEU:HG	0.65	1.68	10	5
1:A:161:VAL:HG12	1:A:197:PHE:CZ	0.65	2.27	4	2
1:A:237:PHE:CE1	4:A:269:HSI:C26	0.65	2.79	10	1
1:A:114:ILE:HD13	1:A:114:ILE:N	0.64	2.06	5	2
1:A:235:VAL:O	1:A:235:VAL:HG12	0.64	1.92	3	3
1:A:174:PHE:CE2	1:A:180:ILE:HG21	0.64	2.28	12	4
1:A:210:THR:HG22	1:A:240:TYR:OH	0.64	1.93	4	4
1:A:182:ALA:HB3	1:A:215:THR:CG2	0.64	2.23	2	2
1:A:162:VAL:HG22	1:A:196:HIS:CD2	0.63	2.28	4	3
1:A:250:LEU:HD12	1:A:250:LEU:N	0.63	2.07	2	2
1:A:134:ILE:HG22	1:A:138:PHE:CE2	0.63	2.29	6	6
1:A:164:ALA:HB1	1:A:168:HIS:HB3	0.63	1.68	4	2
1:A:141:TRP:CG	1:A:224:LEU:HD11	0.63	2.29	10	3
1:A:220:ILE:HD13	1:A:220:ILE:N	0.63	2.09	6	1
1:A:161:VAL:HG12	1:A:197:PHE:CE1	0.62	2.29	5	1
1:A:118:ILE:HG21	1:A:121:TYR:CE2	0.62	2.29	9	1
1:A:221:GLY:HA2	1:A:224:LEU:HD12	0.62	1.70	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ALA:HB2	1:A:217:VAL:HG22	0.62	1.70	15	3
1:A:159:ILE:HG22	1:A:193:GLY:CA	0.62	2.24	3	2
1:A:145:THR:HG22	1:A:146:PRO:HD2	0.62	1.70	3	4
1:A:182:ALA:HB2	1:A:197:PHE:CD2	0.62	2.29	11	3
1:A:245:ILE:HD12	1:A:245:ILE:N	0.62	2.09	6	1
1:A:241:LYS:O	4:A:269:HSI:H35	0.62	1.94	3	1
1:A:243:VAL:HG11	4:A:269:HSI:H33	0.61	1.70	6	1
1:A:133:ALA:HB1	1:A:213:PHE:CA	0.61	2.24	15	3
1:A:144:VAL:HG11	1:A:255:ILE:CG2	0.61	2.25	4	3
1:A:125:MET:SD	1:A:212:LEU:HD23	0.61	2.36	4	1
1:A:254:ASP:O	1:A:258:ILE:HG23	0.61	1.96	3	14
1:A:213:PHE:CE1	1:A:217:VAL:HG21	0.61	2.30	3	4
1:A:133:ALA:HB3	1:A:212:LEU:HD21	0.61	1.71	2	1
1:A:216:ALA:O	1:A:220:ILE:HD12	0.61	1.95	7	3
1:A:220:ILE:HG22	1:A:224:LEU:CD2	0.61	2.26	7	4
1:A:224:LEU:O	1:A:224:LEU:HD12	0.61	1.94	14	1
1:A:181:LEU:HD22	1:A:240:TYR:CZ	0.61	2.31	5	1
1:A:214:LEU:HD21	1:A:240:TYR:CE1	0.61	2.31	15	1
1:A:121:TYR:CD2	1:A:130:VAL:HG21	0.61	2.31	13	2
1:A:149:PHE:CZ	1:A:224:LEU:HD22	0.60	2.31	4	2
1:A:133:ALA:HB1	1:A:213:PHE:HA	0.60	1.72	6	4
1:A:117:ARG:HH11	1:A:156:MET:N	0.60	1.95	6	1
1:A:116:TYR:CD1	1:A:117:ARG:N	0.60	2.70	7	9
1:A:226:LEU:HD12	1:A:258:ILE:HB	0.60	1.74	8	1
1:A:174:PHE:CZ	1:A:180:ILE:HG21	0.59	2.31	14	2
1:A:112:HIS:HA	1:A:147:LEU:HD22	0.59	1.72	6	3
1:A:235:VAL:HG22	4:A:269:HSI:H30	0.59	1.73	9	2
1:A:181:LEU:HD13	1:A:240:TYR:OH	0.59	1.98	3	1
1:A:138:PHE:CE1	1:A:220:ILE:HD12	0.59	2.33	11	3
1:A:220:ILE:HG22	1:A:224:LEU:HD23	0.59	1.75	7	4
1:A:152:ILE:HD11	1:A:157:ALA:HA	0.59	1.74	12	1
1:A:174:PHE:CZ	1:A:180:ILE:CG2	0.58	2.86	14	3
1:A:159:ILE:O	1:A:159:ILE:HD12	0.58	1.97	12	1
1:A:174:PHE:CE2	1:A:180:ILE:CD1	0.58	2.85	1	1
1:A:250:LEU:N	1:A:250:LEU:HD12	0.58	2.13	3	1
1:A:182:ALA:CB	1:A:215:THR:HG21	0.58	2.27	2	1
1:A:181:LEU:HD11	1:A:210:THR:CB	0.58	2.28	7	1
1:A:159:ILE:HD12	1:A:159:ILE:O	0.58	1.97	2	1
1:A:214:LEU:HD11	4:A:269:HSI:C25	0.58	2.29	3	3
1:A:145:THR:HG23	1:A:259:GLN:CB	0.58	2.29	3	3
1:A:224:LEU:CD1	1:A:258:ILE:HD12	0.58	2.28	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:VAL:HG21	1:A:248:PHE:CE1	0.57	2.34	2	1
1:A:211:ASN:H	1:A:211:ASN:ND2	0.57	1.97	12	3
1:A:119:ASN:OD1	1:A:162:VAL:HG22	0.57	1.98	8	1
1:A:141:TRP:O	1:A:145:THR:HG23	0.57	1.99	10	6
1:A:137:ALA:HB1	1:A:220:ILE:CD1	0.57	2.30	8	3
1:A:115:THR:C	1:A:157:ALA:HB1	0.57	2.20	15	1
1:A:214:LEU:C	1:A:214:LEU:HD12	0.57	2.19	3	1
1:A:146:PRO:O	1:A:147:LEU:HD23	0.57	1.99	14	3
1:A:163:PHE:CE2	1:A:197:PHE:CD2	0.57	2.93	7	1
1:A:217:VAL:HG11	1:A:248:PHE:CZ	0.57	2.35	5	3
1:A:174:PHE:CE2	1:A:183:HIS:CE1	0.57	2.93	14	1
1:A:149:PHE:CE1	1:A:224:LEU:HD22	0.57	2.34	4	2
1:A:116:TYR:N	1:A:116:TYR:CD1	0.57	2.73	14	3
1:A:163:PHE:CD2	1:A:197:PHE:CD1	0.57	2.92	4	1
1:A:181:LEU:HD13	1:A:240:TYR:CE2	0.56	2.35	8	3
1:A:198:ASP:O	1:A:198:ASP:CG	0.56	2.43	9	2
1:A:181:LEU:HD13	1:A:240:TYR:CZ	0.56	2.34	15	3
1:A:144:VAL:HG23	1:A:258:ILE:HD11	0.56	1.76	1	5
1:A:160:LEU:HD23	1:A:194:ASP:HB3	0.56	1.76	5	1
1:A:144:VAL:HG23	1:A:145:THR:HG23	0.56	1.77	7	1
1:A:237:PHE:CE1	4:A:269:HSI:C27	0.56	2.88	10	2
1:A:241:LYS:HD3	4:A:269:HSI:H33	0.56	1.77	3	1
1:A:130:VAL:O	1:A:134:ILE:HG23	0.56	2.00	9	1
1:A:180:ILE:HG13	4:A:269:HSI:H402	0.56	1.77	13	1
1:A:184:ALA:CB	1:A:195:ALA:HB2	0.56	2.31	6	1
1:A:119:ASN:HB2	1:A:162:VAL:HG13	0.56	1.78	5	1
1:A:116:TYR:CE2	1:A:151:LYS:HB2	0.56	2.36	14	2
1:A:166:GLY:O	1:A:167:ALA:HB3	0.56	2.00	7	7
1:A:140:VAL:CG1	1:A:250:LEU:HD21	0.55	2.31	2	1
1:A:181:LEU:HD21	1:A:215:THR:CG2	0.55	2.25	6	1
1:A:204:THR:HG21	1:A:208:GLY:O	0.55	2.01	15	2
1:A:126:ASN:H	1:A:205:THR:HG21	0.55	1.61	15	1
1:A:217:VAL:HG11	1:A:248:PHE:HE1	0.55	1.61	9	2
1:A:228:HIS:CD2	1:A:236:MET:O	0.55	2.60	13	10
1:A:235:VAL:HG22	1:A:248:PHE:CZ	0.55	2.36	5	1
1:A:122:THR:HG22	1:A:163:PHE:CZ	0.55	2.37	1	1
1:A:243:VAL:HG11	4:A:269:HSI:C32	0.55	2.32	12	1
1:A:197:PHE:CE2	1:A:215:THR:HG21	0.55	2.37	9	1
1:A:152:ILE:HD12	1:A:154:THR:O	0.55	2.01	8	1
1:A:174:PHE:CZ	1:A:183:HIS:CD2	0.54	2.95	5	3
1:A:214:LEU:HD11	4:A:269:HSI:C19	0.54	2.26	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:269:HSI:O4	4:A:269:HSI:C14	0.54	2.55	13	1
1:A:179:GLY:O	1:A:240:TYR:CD2	0.54	2.60	4	1
1:A:252:ALA:HB1	1:A:256:ARG:HD2	0.54	1.79	10	5
1:A:179:GLY:O	1:A:240:TYR:CE2	0.54	2.61	7	3
1:A:217:VAL:HG11	1:A:248:PHE:CE1	0.54	2.37	9	3
1:A:115:THR:CG2	1:A:152:ILE:HD11	0.54	2.31	6	1
1:A:241:LYS:HB3	4:A:269:HSI:H35	0.54	1.78	14	1
1:A:122:THR:HG23	1:A:163:PHE:CE1	0.54	2.37	2	1
1:A:181:LEU:CD2	1:A:203:TRP:CH2	0.54	2.91	4	1
1:A:213:PHE:CD1	1:A:213:PHE:C	0.54	2.80	14	6
1:A:196:HIS:CD2	1:A:196:HIS:C	0.54	2.81	12	2
1:A:125:MET:CE	1:A:203:TRP:CD1	0.54	2.91	3	1
4:A:269:HSI:O4	4:A:269:HSI:C11	0.54	2.55	11	1
1:A:243:VAL:HG22	1:A:243:VAL:O	0.54	2.02	9	1
1:A:130:VAL:HG11	1:A:163:PHE:CE2	0.54	2.38	10	1
1:A:235:VAL:CG2	1:A:248:PHE:CE1	0.54	2.91	4	1
1:A:115:THR:C	1:A:116:TYR:CD1	0.53	2.81	2	1
1:A:117:ARG:HB3	1:A:157:ALA:HB3	0.53	1.79	12	2
1:A:133:ALA:CB	1:A:212:LEU:HD12	0.53	2.32	7	1
1:A:130:VAL:HG22	1:A:212:LEU:HG	0.53	1.81	15	1
1:A:138:PHE:CE1	1:A:149:PHE:CG	0.53	2.96	5	2
1:A:241:LYS:HD2	4:A:269:HSI:H33	0.53	1.80	12	1
1:A:163:PHE:CD2	1:A:197:PHE:CE1	0.53	2.97	4	1
1:A:179:GLY:C	1:A:180:ILE:HD12	0.53	2.24	12	1
1:A:213:PHE:C	1:A:213:PHE:CD1	0.53	2.81	7	2
1:A:179:GLY:O	1:A:180:ILE:HD12	0.53	2.03	12	1
1:A:114:ILE:HD12	1:A:224:LEU:CD2	0.53	2.34	12	1
1:A:115:THR:HG21	1:A:152:ILE:HD11	0.53	1.80	6	1
1:A:145:THR:HG23	1:A:259:GLN:HB3	0.53	1.81	9	1
1:A:114:ILE:HG21	1:A:149:PHE:CZ	0.53	2.38	8	1
1:A:229:SER:HB3	1:A:234:ALA:HB2	0.53	1.81	2	1
1:A:212:LEU:HD13	1:A:212:LEU:O	0.53	2.04	1	2
1:A:217:VAL:HG21	1:A:248:PHE:CE1	0.53	2.38	10	1
1:A:183:HIS:ND1	1:A:183:HIS:N	0.53	2.57	14	2
1:A:214:LEU:CD1	4:A:269:HSI:H19	0.53	2.25	15	1
1:A:235:VAL:CG2	1:A:248:PHE:CD1	0.53	2.92	4	1
1:A:163:PHE:CD1	1:A:197:PHE:CD2	0.53	2.97	10	1
1:A:222:HIS:CE1	1:A:228:HIS:CE1	0.53	2.96	3	3
1:A:195:ALA:HB2	1:A:219:GLU:HB2	0.53	1.80	7	1
1:A:122:THR:HG21	1:A:199:GLU:OE1	0.52	2.04	5	1
1:A:137:ALA:CB	1:A:220:ILE:HD12	0.52	2.35	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:TYR:CD1	1:A:241:LYS:N	0.52	2.78	7	3
1:A:163:PHE:CE1	1:A:197:PHE:CE2	0.52	2.97	10	1
1:A:175:ASP:HB3	1:A:180:ILE:HD12	0.52	1.81	2	1
1:A:116:TYR:C	1:A:116:TYR:CD1	0.52	2.82	5	1
1:A:181:LEU:CD1	1:A:203:TRP:CZ3	0.52	2.93	5	1
1:A:113:TYR:C	1:A:114:ILE:HD13	0.52	2.25	8	2
4:A:269:HSI:C13	4:A:269:HSI:C3	0.52	2.87	13	1
1:A:145:THR:HG23	1:A:259:GLN:HA	0.52	1.81	3	3
1:A:237:PHE:HE1	4:A:269:HSI:C27	0.52	2.17	15	2
1:A:115:THR:O	1:A:158:ASP:N	0.52	2.43	15	1
1:A:137:ALA:HB1	1:A:220:ILE:HD12	0.51	1.83	3	1
1:A:197:PHE:CD1	1:A:197:PHE:N	0.51	2.78	15	4
1:A:203:TRP:CZ3	1:A:212:LEU:HD22	0.51	2.39	4	1
1:A:119:ASN:HB3	1:A:163:PHE:CZ	0.51	2.39	15	2
1:A:141:TRP:CD1	1:A:220:ILE:CG2	0.51	2.94	2	4
1:A:133:ALA:HB1	1:A:213:PHE:N	0.51	2.21	4	2
1:A:238:PRO:O	4:A:269:HSI:H14	0.51	2.05	10	1
1:A:211:ASN:OD1	1:A:214:LEU:HD23	0.51	2.05	11	1
1:A:183:HIS:N	1:A:183:HIS:HD1	0.51	2.04	14	1
1:A:174:PHE:CE1	1:A:180:ILE:HG21	0.51	2.41	3	1
1:A:140:VAL:O	1:A:144:VAL:CG2	0.51	2.59	4	10
1:A:232:PRO:HA	1:A:237:PHE:CD2	0.51	2.41	6	3
1:A:231:ASP:O	1:A:234:ALA:HB3	0.51	2.05	14	1
1:A:197:PHE:N	1:A:197:PHE:CD1	0.51	2.74	10	5
1:A:116:TYR:CE2	1:A:151:LYS:HD2	0.51	2.41	12	1
1:A:229:SER:CB	1:A:234:ALA:HB3	0.51	2.36	8	2
1:A:117:ARG:NH1	1:A:155:GLY:H	0.51	2.03	6	1
1:A:159:ILE:HD11	1:A:223:SER:HB3	0.51	1.82	11	1
1:A:211:ASN:ND2	1:A:211:ASN:H	0.51	2.04	7	3
1:A:210:THR:HG23	1:A:242:TYR:HB3	0.51	1.83	8	1
1:A:180:ILE:HD13	1:A:180:ILE:N	0.50	2.22	7	1
1:A:141:TRP:O	1:A:145:THR:CG2	0.50	2.59	5	5
1:A:175:ASP:CB	1:A:180:ILE:CG1	0.50	2.89	4	1
1:A:175:ASP:CG	1:A:180:ILE:HG22	0.50	2.25	6	1
1:A:235:VAL:O	1:A:235:VAL:HG13	0.50	2.07	1	1
1:A:122:THR:HG21	1:A:125:MET:HB2	0.50	1.81	2	1
1:A:181:LEU:HB3	1:A:215:THR:HG23	0.50	1.82	2	2
1:A:189:SER:O	1:A:191:ILE:HD12	0.50	2.06	14	1
4:A:269:HSI:O1	4:A:269:HSI:C11	0.50	2.59	1	1
1:A:174:PHE:CE2	1:A:180:ILE:CG2	0.50	2.94	6	2
1:A:188:GLY:O	1:A:192:GLY:HA3	0.50	2.06	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:258:ILE:CG1	1:A:259:GLN:N	0.50	2.75	9	12
1:A:125:MET:CE	1:A:163:PHE:CE2	0.50	2.94	7	1
1:A:119:ASN:HB3	1:A:163:PHE:CE2	0.50	2.42	8	2
1:A:117:ARG:HB3	1:A:160:LEU:HD12	0.50	1.83	3	1
1:A:181:LEU:HD13	1:A:240:TYR:HE2	0.50	1.67	7	1
1:A:178:GLY:O	1:A:179:GLY:C	0.49	2.51	12	2
1:A:116:TYR:CE2	1:A:159:ILE:HG21	0.49	2.41	9	1
1:A:174:PHE:CE1	1:A:180:ILE:HD13	0.49	2.42	3	1
1:A:134:ILE:HD13	1:A:134:ILE:N	0.49	2.22	3	1
1:A:134:ILE:HD11	1:A:212:LEU:HD11	0.49	1.84	3	1
1:A:180:ILE:HG22	1:A:181:LEU:N	0.49	2.22	2	3
1:A:122:THR:N	1:A:125:MET:O	0.49	2.46	15	2
1:A:180:ILE:HA	4:A:269:HSI:H402	0.49	1.85	14	1
1:A:182:ALA:CB	1:A:197:PHE:CD2	0.49	2.96	3	2
1:A:232:PRO:HB3	1:A:239:THR:HG21	0.49	1.83	12	1
1:A:163:PHE:CD2	1:A:197:PHE:HB3	0.49	2.42	7	1
1:A:140:VAL:HG13	1:A:250:LEU:HD11	0.49	1.84	8	1
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.49	2.43	5	5
1:A:113:TYR:O	1:A:113:TYR:CD2	0.49	2.65	5	2
1:A:204:THR:HG21	1:A:208:GLY:HA3	0.49	1.83	4	1
1:A:181:LEU:HD22	1:A:240:TYR:HE1	0.49	1.65	15	1
1:A:217:VAL:HG11	1:A:248:PHE:HZ	0.49	1.67	5	2
1:A:182:ALA:HB1	1:A:196:HIS:O	0.49	2.06	7	1
1:A:243:VAL:CG1	4:A:269:HSI:C33	0.49	2.83	6	1
1:A:140:VAL:O	1:A:143:ASN:ND2	0.49	2.45	7	14
1:A:235:VAL:O	4:A:269:HSI:C28	0.49	2.54	5	1
1:A:235:VAL:HG21	1:A:248:PHE:CE2	0.49	2.42	12	1
1:A:235:VAL:HA	4:A:269:HSI:H30	0.49	1.84	8	2
1:A:181:LEU:HD11	1:A:210:THR:HB	0.49	1.85	7	1
1:A:182:ALA:CB	1:A:196:HIS:O	0.49	2.61	7	1
1:A:118:ILE:HD11	1:A:134:ILE:HD11	0.49	1.84	6	1
1:A:243:VAL:CG2	1:A:243:VAL:O	0.49	2.61	9	1
1:A:116:TYR:CE2	1:A:138:PHE:CE1	0.49	3.01	10	1
1:A:116:TYR:CD2	1:A:151:LYS:HB2	0.48	2.43	14	2
1:A:204:THR:HG21	1:A:208:GLY:C	0.48	2.28	1	1
1:A:181:LEU:O	1:A:182:ALA:HB2	0.48	2.08	10	1
1:A:235:VAL:HG21	1:A:248:PHE:HE1	0.48	1.67	1	1
1:A:199:GLU:HA	1:A:203:TRP:CZ2	0.48	2.44	11	1
1:A:250:LEU:HD12	1:A:250:LEU:H	0.48	1.66	4	1
1:A:118:ILE:HD13	1:A:161:VAL:HG23	0.48	1.85	6	1
1:A:174:PHE:CD1	1:A:174:PHE:N	0.48	2.82	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:LEU:HD21	1:A:214:LEU:HG	0.48	1.84	10	1
1:A:249:ARG:NE	1:A:250:LEU:O	0.48	2.46	10	13
1:A:213:PHE:CZ	1:A:217:VAL:HG21	0.48	2.43	12	1
1:A:140:VAL:HG11	1:A:250:LEU:HD11	0.48	1.85	8	1
1:A:216:ALA:O	1:A:220:ILE:CG1	0.48	2.61	4	4
1:A:116:TYR:C	1:A:157:ALA:CB	0.48	2.82	2	1
1:A:226:LEU:HD11	1:A:258:ILE:HG22	0.48	1.84	4	1
1:A:245:ILE:O	1:A:248:PHE:CD1	0.48	2.67	12	1
1:A:139:GLN:O	1:A:143:ASN:ND2	0.48	2.47	4	14
1:A:183:HIS:CE1	1:A:196:HIS:HB2	0.48	2.44	14	3
1:A:239:THR:HG22	1:A:239:THR:O	0.48	2.08	12	1
1:A:117:ARG:N	1:A:159:ILE:O	0.48	2.47	7	2
1:A:221:GLY:O	1:A:225:GLY:N	0.48	2.47	4	4
1:A:213:PHE:HB3	1:A:245:ILE:HD11	0.48	1.85	9	1
1:A:196:HIS:C	1:A:196:HIS:CD2	0.48	2.87	3	1
1:A:117:ARG:C	1:A:117:ARG:CD	0.48	2.82	2	1
1:A:163:PHE:CE2	1:A:197:PHE:CE1	0.48	3.02	4	1
1:A:174:PHE:CZ	1:A:180:ILE:CD1	0.48	2.97	11	1
1:A:125:MET:HE1	1:A:203:TRP:CD1	0.48	2.44	3	1
1:A:244:ASP:OD1	1:A:247:THR:HG23	0.47	2.09	2	1
1:A:138:PHE:CD1	1:A:149:PHE:CD1	0.47	3.02	3	2
1:A:237:PHE:CE1	1:A:239:THR:O	0.47	2.67	15	3
1:A:224:LEU:HD12	1:A:225:GLY:H	0.47	1.62	7	2
1:A:181:LEU:HD21	1:A:210:THR:HG21	0.47	1.84	1	1
1:A:235:VAL:HG12	1:A:235:VAL:O	0.47	2.08	11	1
1:A:146:PRO:C	1:A:147:LEU:HD23	0.47	2.30	14	2
1:A:248:PHE:CD1	1:A:248:PHE:C	0.47	2.88	12	1
1:A:239:THR:O	4:A:269:HSI:H16	0.47	2.09	10	1
1:A:197:PHE:HB3	1:A:203:TRP:CZ2	0.47	2.44	3	1
1:A:213:PHE:CD1	1:A:245:ILE:HG12	0.47	2.45	13	5
1:A:181:LEU:HD21	1:A:211:ASN:O	0.47	2.09	2	2
1:A:116:TYR:CE2	1:A:159:ILE:HD12	0.47	2.45	10	1
1:A:160:LEU:CD1	1:A:162:VAL:HG12	0.47	2.40	10	1
1:A:118:ILE:O	1:A:119:ASN:C	0.47	2.53	4	5
1:A:244:ASP:OD1	1:A:244:ASP:C	0.47	2.52	6	1
1:A:161:VAL:HG22	1:A:197:PHE:CZ	0.47	2.43	11	1
1:A:217:VAL:HG21	1:A:248:PHE:CZ	0.47	2.44	11	2
1:A:142:SER:OG	1:A:149:PHE:CD2	0.47	2.67	4	1
1:A:250:LEU:CD1	1:A:250:LEU:N	0.47	2.75	7	4
1:A:164:ALA:O	1:A:199:GLU:N	0.47	2.46	11	1
1:A:183:HIS:O	1:A:195:ALA:HB1	0.47	2.10	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:VAL:HG22	1:A:248:PHE:CE1	0.47	2.44	4	1
1:A:114:ILE:N	1:A:148:LYS:O	0.47	2.46	7	1
1:A:220:ILE:CG2	1:A:224:LEU:HD21	0.47	2.40	1	1
1:A:116:TYR:CD1	1:A:116:TYR:N	0.47	2.82	10	1
1:A:132:TYR:O	1:A:136:LYS:CE	0.47	2.63	10	1
1:A:159:ILE:CD1	1:A:159:ILE:O	0.47	2.63	2	2
1:A:245:ILE:N	1:A:245:ILE:CD1	0.47	2.75	6	1
1:A:152:ILE:HD12	1:A:154:THR:CG2	0.47	2.36	5	1
1:A:235:VAL:O	1:A:236:MET:CG	0.47	2.64	1	3
1:A:221:GLY:O	1:A:225:GLY:CA	0.47	2.63	4	2
1:A:212:LEU:O	1:A:212:LEU:HD13	0.47	2.09	3	2
1:A:125:MET:SD	1:A:163:PHE:CZ	0.47	3.08	7	1
1:A:234:ALA:O	1:A:237:PHE:CD2	0.47	2.67	7	3
1:A:247:THR:O	4:A:269:HSI:CL1	0.46	2.70	14	1
1:A:213:PHE:CD1	1:A:245:ILE:CG1	0.46	2.98	15	1
1:A:229:SER:CB	1:A:234:ALA:HB1	0.46	2.40	14	1
1:A:222:HIS:N	1:A:236:MET:HE3	0.46	2.25	9	1
1:A:130:VAL:O	1:A:134:ILE:CG1	0.46	2.63	4	7
1:A:244:ASP:O	1:A:245:ILE:CB	0.46	2.64	3	2
1:A:129:ASP:N	1:A:129:ASP:OD1	0.46	2.49	4	1
1:A:181:LEU:HD12	1:A:201:GLU:OE1	0.46	2.10	9	1
1:A:116:TYR:CD2	1:A:138:PHE:CE2	0.46	3.04	4	1
1:A:174:PHE:CE2	1:A:180:ILE:HD13	0.46	2.46	1	1
1:A:174:PHE:CE2	1:A:180:ILE:HG22	0.46	2.46	9	1
1:A:133:ALA:CB	1:A:212:LEU:CD2	0.46	2.92	2	1
1:A:198:ASP:OD2	1:A:198:ASP:O	0.46	2.33	11	1
1:A:180:ILE:CD1	1:A:182:ALA:N	0.46	2.78	5	1
1:A:166:GLY:O	1:A:167:ALA:HB2	0.46	2.11	10	1
1:A:232:PRO:HA	1:A:237:PHE:CE2	0.46	2.45	6	3
1:A:218:HIS:CE1	1:A:236:MET:O	0.46	2.68	12	2
1:A:149:PHE:CZ	1:A:224:LEU:CD2	0.46	2.99	10	1
1:A:218:HIS:CD2	1:A:236:MET:CE	0.46	2.99	14	1
1:A:129:ASP:OD2	1:A:205:THR:HG22	0.46	2.11	15	1
1:A:235:VAL:O	1:A:235:VAL:CG1	0.46	2.63	3	1
1:A:180:ILE:HG23	1:A:198:ASP:OD2	0.46	2.10	3	1
1:A:181:LEU:HD22	1:A:203:TRP:CH2	0.46	2.46	4	1
1:A:243:VAL:HG13	1:A:243:VAL:O	0.46	2.11	15	2
1:A:147:LEU:O	1:A:149:PHE:CE1	0.46	2.69	3	2
1:A:180:ILE:CG2	1:A:198:ASP:OD2	0.46	2.64	3	1
1:A:116:TYR:N	1:A:157:ALA:HB1	0.46	2.26	8	1
1:A:181:LEU:HD21	1:A:210:THR:CB	0.46	2.40	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:HIS:C	1:A:183:HIS:ND1	0.46	2.69	15	2
1:A:122:THR:HG23	1:A:124:ASP:H	0.46	1.71	8	1
1:A:158:ASP:OD1	1:A:158:ASP:N	0.46	2.45	6	1
1:A:122:THR:HG23	1:A:123:PRO:CD	0.46	2.41	15	1
1:A:181:LEU:CD1	1:A:203:TRP:CH2	0.45	2.97	5	1
1:A:141:TRP:CE3	1:A:224:LEU:CD1	0.45	2.99	5	1
1:A:118:ILE:O	1:A:118:ILE:CG2	0.45	2.64	5	2
1:A:243:VAL:O	1:A:243:VAL:HG13	0.45	2.11	12	1
1:A:121:TYR:C	1:A:122:THR:HG22	0.45	2.31	15	1
1:A:121:TYR:O	1:A:163:PHE:CD2	0.45	2.69	10	1
1:A:145:THR:HG23	1:A:259:GLN:CA	0.45	2.40	3	3
1:A:216:ALA:O	1:A:220:ILE:CD1	0.45	2.64	7	2
1:A:163:PHE:CD2	1:A:197:PHE:CB	0.45	2.99	7	1
1:A:226:LEU:HD21	1:A:258:ILE:HA	0.45	1.87	6	1
1:A:121:TYR:C	1:A:122:THR:HG23	0.45	2.31	1	1
1:A:228:HIS:CE1	1:A:236:MET:CE	0.45	2.99	3	2
1:A:114:ILE:HG13	1:A:149:PHE:CE2	0.45	2.46	5	1
1:A:154:THR:HG23	1:A:155:GLY:N	0.45	2.27	5	1
1:A:180:ILE:N	1:A:180:ILE:HD13	0.45	2.26	4	1
1:A:252:ALA:HA	1:A:255:ILE:HD11	0.45	1.89	8	2
1:A:168:HIS:O	1:A:168:HIS:CD2	0.45	2.69	12	1
1:A:206:HIS:O	1:A:207:SER:CB	0.45	2.64	7	2
1:A:235:VAL:CG2	1:A:248:PHE:CE2	0.45	3.00	5	1
1:A:141:TRP:CE3	1:A:224:LEU:HD12	0.45	2.46	5	1
1:A:213:PHE:CE1	1:A:245:ILE:CG2	0.45	2.98	12	1
1:A:114:ILE:HD12	1:A:224:LEU:HD22	0.45	1.88	12	1
1:A:205:THR:O	1:A:206:HIS:CB	0.45	2.65	3	3
1:A:118:ILE:HG12	1:A:121:TYR:CE2	0.45	2.45	13	1
1:A:138:PHE:CE1	1:A:149:PHE:CB	0.45	3.00	15	2
1:A:240:TYR:C	1:A:240:TYR:CD1	0.45	2.90	5	2
1:A:174:PHE:CZ	1:A:183:HIS:ND1	0.45	2.84	14	1
1:A:194:ASP:N	1:A:194:ASP:OD1	0.45	2.50	7	2
1:A:121:TYR:O	1:A:122:THR:HG22	0.45	2.12	15	1
1:A:145:THR:HB	1:A:147:LEU:HD12	0.45	1.89	8	1
1:A:141:TRP:CZ2	1:A:221:GLY:HA3	0.45	2.47	2	2
1:A:222:HIS:CG	1:A:236:MET:CE	0.45	3.00	2	1
1:A:240:TYR:HA	4:A:269:HSI:C25	0.45	2.42	2	1
1:A:136:LYS:HB3	1:A:213:PHE:CD1	0.45	2.47	4	1
1:A:125:MET:CE	1:A:163:PHE:CZ	0.45	2.99	15	1
4:A:269:HSI:C44	4:A:269:HSI:C3	0.45	2.95	10	1
1:A:212:LEU:HD13	1:A:212:LEU:C	0.45	2.32	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:213:PHE:CE1	1:A:217:VAL:CG2	0.45	3.00	5	3
1:A:228:HIS:ND1	1:A:228:HIS:N	0.45	2.64	4	1
1:A:114:ILE:CG1	1:A:149:PHE:CE1	0.45	2.99	8	1
1:A:141:TRP:CD2	1:A:224:LEU:CD1	0.45	3.00	8	2
1:A:245:ILE:H	1:A:245:ILE:HD12	0.45	1.71	15	2
1:A:152:ILE:HD11	1:A:155:GLY:O	0.45	2.12	10	1
1:A:138:PHE:CE1	1:A:149:PHE:CD2	0.45	3.05	8	1
1:A:143:ASN:HD21	1:A:144:VAL:HG13	0.44	1.70	4	9
1:A:122:THR:HG22	1:A:123:PRO:HD2	0.44	1.88	5	3
1:A:245:ILE:H	1:A:245:ILE:CD1	0.44	2.23	6	1
1:A:235:VAL:HG23	1:A:249:ARG:O	0.44	2.12	15	1
1:A:133:ALA:HB3	1:A:212:LEU:CD1	0.44	2.41	10	1
1:A:214:LEU:HD11	4:A:269:HSI:C26	0.44	2.41	3	1
1:A:180:ILE:CG1	4:A:269:HSI:H402	0.44	2.42	13	1
1:A:214:LEU:CD1	4:A:269:HSI:C26	0.44	2.95	5	2
1:A:114:ILE:HB	1:A:149:PHE:CD2	0.44	2.47	5	1
1:A:223:SER:O	1:A:224:LEU:C	0.44	2.55	9	1
1:A:154:THR:HG23	1:A:154:THR:O	0.44	2.13	2	1
1:A:118:ILE:CG2	1:A:118:ILE:O	0.44	2.66	11	2
1:A:114:ILE:N	1:A:114:ILE:CD1	0.44	2.73	5	1
1:A:213:PHE:CE1	1:A:248:PHE:CD2	0.44	3.05	7	1
1:A:121:TYR:CD2	1:A:127:ARG:HG2	0.44	2.47	5	2
1:A:164:ALA:HB1	1:A:168:HIS:CB	0.44	2.42	4	1
1:A:226:LEU:N	1:A:226:LEU:HD13	0.44	2.28	13	1
1:A:237:PHE:CE2	1:A:239:THR:HB	0.44	2.48	11	3
1:A:124:ASP:OD1	1:A:124:ASP:N	0.44	2.51	11	1
1:A:197:PHE:CB	1:A:203:TRP:CZ2	0.44	3.00	4	1
1:A:166:GLY:O	1:A:167:ALA:CB	0.44	2.65	7	2
4:A:269:HSI:H402	4:A:269:HSI:C14	0.44	2.42	6	1
1:A:222:HIS:N	1:A:236:MET:CE	0.44	2.81	9	1
1:A:183:HIS:ND1	1:A:183:HIS:C	0.44	2.71	2	3
1:A:197:PHE:HB2	1:A:203:TRP:CZ2	0.44	2.48	11	1
1:A:181:LEU:CG	1:A:215:THR:HG23	0.44	2.43	5	1
1:A:152:ILE:HD11	1:A:157:ALA:CA	0.44	2.42	12	1
1:A:116:TYR:CE2	1:A:159:ILE:CG2	0.44	3.01	9	1
1:A:119:ASN:ND2	1:A:162:VAL:HG13	0.44	2.27	9	1
1:A:159:ILE:HD12	1:A:220:ILE:HD13	0.44	1.89	11	1
1:A:183:HIS:O	1:A:195:ALA:CB	0.44	2.65	3	3
1:A:235:VAL:O	1:A:236:MET:CB	0.44	2.66	3	2
1:A:119:ASN:ND2	1:A:162:VAL:HG22	0.44	2.28	1	1
1:A:122:THR:HG22	1:A:163:PHE:CE1	0.44	2.47	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:HIS:CB	1:A:146:PRO:O	0.44	2.66	3	1
1:A:238:PRO:O	4:A:269:HSI:C16	0.43	2.66	4	1
1:A:114:ILE:HG22	1:A:158:ASP:OD2	0.43	2.13	8	1
1:A:249:ARG:C	1:A:250:LEU:HD13	0.43	2.34	11	2
1:A:180:ILE:HD12	1:A:182:ALA:N	0.43	2.28	5	1
1:A:157:ALA:HB3	1:A:160:LEU:CD1	0.43	2.44	1	2
1:A:211:ASN:ND2	1:A:211:ASN:N	0.43	2.66	12	2
1:A:225:GLY:O	1:A:226:LEU:HD12	0.43	2.14	10	1
1:A:116:TYR:CE1	1:A:149:PHE:HB3	0.43	2.48	10	1
1:A:235:VAL:HG13	1:A:248:PHE:CZ	0.43	2.48	8	1
1:A:159:ILE:O	1:A:159:ILE:CG1	0.43	2.66	2	2
1:A:181:LEU:HD21	1:A:210:THR:HB	0.43	1.91	11	1
1:A:144:VAL:O	1:A:258:ILE:CG1	0.43	2.66	4	1
1:A:160:LEU:HB2	1:A:194:ASP:CG	0.43	2.33	1	1
1:A:174:PHE:CD2	1:A:196:HIS:NE2	0.43	2.86	3	1
1:A:152:ILE:HD12	1:A:155:GLY:H	0.43	1.73	2	1
1:A:224:LEU:CD1	1:A:225:GLY:N	0.43	2.78	11	3
1:A:161:VAL:CG1	1:A:197:PHE:CZ	0.43	3.01	4	1
1:A:186:GLY:O	1:A:192:GLY:CA	0.43	2.66	10	1
1:A:165:ARG:CD	1:A:165:ARG:N	0.43	2.82	11	1
1:A:228:HIS:CG	1:A:236:MET:O	0.43	2.71	4	1
1:A:219:GLU:CG	1:A:220:ILE:N	0.43	2.82	8	1
1:A:179:GLY:O	1:A:180:ILE:CB	0.43	2.64	14	1
1:A:116:TYR:CE2	1:A:151:LYS:CD	0.43	3.01	12	1
1:A:178:GLY:O	1:A:180:ILE:N	0.43	2.51	7	1
1:A:149:PHE:HE2	1:A:159:ILE:HD12	0.43	1.73	8	1
1:A:229:SER:OG	1:A:234:ALA:HB3	0.43	2.14	8	1
1:A:181:LEU:HD21	1:A:210:THR:CG2	0.43	2.43	11	1
1:A:114:ILE:HD11	1:A:147:LEU:HD13	0.43	1.91	11	1
1:A:213:PHE:CD2	1:A:245:ILE:HG12	0.43	2.49	4	1
1:A:118:ILE:HG22	1:A:118:ILE:O	0.43	2.13	4	1
1:A:250:LEU:H	1:A:250:LEU:HD22	0.43	1.72	7	1
1:A:197:PHE:HB3	1:A:203:TRP:CH2	0.43	2.49	15	1
1:A:115:THR:CG2	1:A:152:ILE:HG23	0.43	2.44	13	1
1:A:120:ASN:O	1:A:121:TYR:CD1	0.43	2.72	2	1
1:A:144:VAL:CG1	1:A:255:ILE:CG2	0.43	2.95	4	1
1:A:181:LEU:O	1:A:197:PHE:CD1	0.43	2.72	7	1
1:A:114:ILE:CG2	1:A:159:ILE:HD11	0.43	2.44	6	1
1:A:174:PHE:CD1	1:A:180:ILE:HG21	0.43	2.49	3	1
1:A:121:TYR:CE2	1:A:130:VAL:HG21	0.43	2.49	13	1
1:A:220:ILE:N	1:A:220:ILE:CD1	0.43	2.77	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:PHE:CE1	1:A:220:ILE:HD13	0.42	2.47	14	1
1:A:224:LEU:CD1	1:A:225:GLY:H	0.42	2.26	7	1
1:A:243:VAL:O	1:A:243:VAL:HG22	0.42	2.13	10	2
1:A:116:TYR:CD2	1:A:159:ILE:HG12	0.42	2.49	2	1
1:A:118:ILE:HG23	1:A:118:ILE:O	0.42	2.14	11	1
1:A:211:ASN:ND2	1:A:245:ILE:HD11	0.42	2.28	10	1
4:A:269:HSI:H401	4:A:269:HSI:C14	0.42	2.43	11	1
1:A:180:ILE:HD12	1:A:181:LEU:N	0.42	2.28	5	1
1:A:175:ASP:CG	1:A:176:GLY:N	0.42	2.73	8	1
1:A:116:TYR:OH	1:A:161:VAL:HG21	0.42	2.14	1	2
1:A:186:GLY:N	1:A:187:PRO:CD	0.42	2.83	15	2
4:A:269:HSI:H14	4:A:269:HSI:C40	0.42	2.44	6	1
1:A:201:GLU:HG3	1:A:202:PHE:N	0.42	2.29	1	2
1:A:122:THR:N	1:A:123:PRO:HD2	0.42	2.29	9	1
1:A:116:TYR:CD2	1:A:159:ILE:CG1	0.42	3.02	2	1
1:A:138:PHE:CE1	1:A:149:PHE:HB2	0.42	2.49	11	2
1:A:144:VAL:O	1:A:258:ILE:HD11	0.42	2.14	4	1
1:A:125:MET:SD	1:A:163:PHE:CE2	0.42	3.12	7	1
1:A:141:TRP:CD1	1:A:220:ILE:HG21	0.42	2.49	9	1
1:A:182:ALA:HB3	1:A:219:GLU:OE2	0.42	2.14	11	1
1:A:237:PHE:CG	1:A:238:PRO:HD2	0.42	2.50	4	1
1:A:197:PHE:CZ	1:A:219:GLU:CG	0.42	3.03	12	1
1:A:248:PHE:CD2	1:A:248:PHE:O	0.42	2.73	7	1
1:A:226:LEU:HD22	1:A:227:GLY:N	0.42	2.30	13	1
1:A:197:PHE:HB2	1:A:203:TRP:CH2	0.42	2.49	11	1
1:A:160:LEU:O	1:A:195:ALA:N	0.42	2.53	11	1
1:A:240:TYR:CD1	1:A:240:TYR:C	0.42	2.93	11	2
1:A:125:MET:HE1	1:A:203:TRP:CD2	0.42	2.50	4	1
1:A:137:ALA:CB	1:A:217:VAL:HG23	0.42	2.45	7	1
1:A:219:GLU:OE2	1:A:220:ILE:HG23	0.42	2.14	15	1
1:A:212:LEU:CD1	1:A:212:LEU:C	0.42	2.85	7	1
1:A:119:ASN:O	1:A:121:TYR:N	0.42	2.53	1	1
1:A:197:PHE:CE2	1:A:215:THR:CG2	0.42	3.02	9	1
1:A:184:ALA:HB3	1:A:222:HIS:CB	0.42	2.45	10	1
1:A:181:LEU:HD22	1:A:215:THR:OG1	0.42	2.15	4	1
1:A:226:LEU:H	1:A:226:LEU:HD12	0.42	1.75	7	1
1:A:218:HIS:HD1	4:A:269:HSI:C19	0.42	2.27	6	1
1:A:174:PHE:CZ	1:A:180:ILE:HG22	0.42	2.49	9	1
1:A:237:PHE:CD1	1:A:239:THR:HB	0.42	2.49	8	1
1:A:235:VAL:CG2	1:A:248:PHE:CZ	0.41	3.03	2	1
1:A:165:ARG:CD	1:A:165:ARG:H	0.41	2.28	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:PHE:CD1	1:A:149:PHE:N	0.41	2.88	3	2
1:A:243:VAL:O	1:A:243:VAL:CG2	0.41	2.68	6	2
1:A:228:HIS:HD1	1:A:228:HIS:N	0.41	2.13	3	1
1:A:235:VAL:HG13	4:A:269:HSI:H28	0.41	1.91	11	1
1:A:116:TYR:CD2	1:A:138:PHE:CZ	0.41	3.08	4	1
1:A:252:ALA:O	1:A:256:ARG:CG	0.41	2.68	4	1
1:A:121:TYR:N	1:A:121:TYR:CD1	0.41	2.86	4	1
1:A:140:VAL:HG21	1:A:250:LEU:HD11	0.41	1.92	7	1
1:A:174:PHE:CD2	1:A:180:ILE:HG12	0.41	2.49	1	1
1:A:139:GLN:HG2	1:A:140:VAL:N	0.41	2.30	15	2
1:A:168:HIS:ND1	1:A:168:HIS:N	0.41	2.67	4	1
1:A:116:TYR:CZ	1:A:151:LYS:HD2	0.41	2.51	12	2
1:A:207:SER:C	1:A:244:ASP:OD2	0.41	2.58	10	1
1:A:114:ILE:CG1	1:A:149:PHE:CE2	0.41	3.03	5	1
1:A:136:LYS:CD	1:A:139:GLN:OE1	0.41	2.69	1	1
1:A:111:LYS:N	1:A:111:LYS:CD	0.41	2.83	15	1
1:A:235:VAL:HG21	1:A:250:LEU:HG	0.41	1.91	3	1
1:A:122:THR:HG21	1:A:203:TRP:CH2	0.41	2.51	8	1
1:A:228:HIS:CD2	1:A:236:MET:HE3	0.41	2.51	5	1
1:A:220:ILE:CG2	1:A:224:LEU:HD23	0.41	2.46	14	1
1:A:243:VAL:HG21	1:A:248:PHE:N	0.41	2.30	14	1
1:A:138:PHE:O	1:A:142:SER:CB	0.41	2.68	7	1
1:A:222:HIS:CE1	1:A:227:GLY:O	0.41	2.73	7	1
1:A:213:PHE:CD1	1:A:245:ILE:HG23	0.41	2.49	6	1
1:A:215:THR:HG22	1:A:219:GLU:HG3	0.41	1.92	10	1
1:A:174:PHE:CZ	1:A:180:ILE:HD11	0.41	2.50	1	1
1:A:180:ILE:CD1	1:A:198:ASP:OD2	0.41	2.69	1	1
1:A:182:ALA:O	4:A:269:HSI:H402	0.41	2.16	4	1
1:A:121:TYR:CD2	1:A:127:ARG:HB3	0.41	2.50	4	1
1:A:182:ALA:HB3	1:A:215:THR:HG22	0.41	1.91	12	1
1:A:235:VAL:CG1	1:A:235:VAL:O	0.41	2.69	7	1
1:A:229:SER:CB	1:A:234:ALA:HB2	0.41	2.45	10	1
1:A:140:VAL:CG1	1:A:250:LEU:CD1	0.41	2.94	8	1
1:A:201:GLU:CG	1:A:202:PHE:N	0.41	2.84	12	2
1:A:182:ALA:HB2	1:A:215:THR:CG2	0.41	2.46	6	1
1:A:229:SER:CB	1:A:234:ALA:CB	0.41	2.98	8	1
1:A:161:VAL:HG12	1:A:161:VAL:O	0.41	2.16	11	1
1:A:203:TRP:HH2	1:A:215:THR:HG21	0.41	1.74	4	1
1:A:258:ILE:HG13	1:A:259:GLN:N	0.41	2.31	7	1
1:A:250:LEU:HD22	1:A:250:LEU:O	0.41	2.16	10	1
1:A:214:LEU:HG	1:A:215:THR:N	0.41	2.29	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ILE:CG1	1:A:157:ALA:HB2	0.41	2.45	8	1
1:A:136:LYS:HB3	1:A:213:PHE:CE1	0.41	2.51	4	1
1:A:181:LEU:HD11	1:A:210:THR:OG1	0.41	2.15	7	1
1:A:121:TYR:O	1:A:163:PHE:CE2	0.41	2.74	10	1
1:A:199:GLU:OE1	1:A:199:GLU:CA	0.40	2.68	13	1
1:A:160:LEU:HD21	1:A:162:VAL:HG11	0.40	1.93	4	1
1:A:185:PHE:O	1:A:193:GLY:N	0.40	2.54	15	1
1:A:159:ILE:HD13	1:A:223:SER:CB	0.40	2.46	10	1
1:A:244:ASP:OD1	1:A:246:ASN:CB	0.40	2.70	10	1
1:A:122:THR:CG2	1:A:125:MET:HB2	0.40	2.46	2	1
1:A:210:THR:HG22	1:A:240:TYR:CZ	0.40	2.50	11	1
1:A:175:ASP:N	1:A:175:ASP:OD1	0.40	2.47	7	1
4:A:269:HSI:C48	4:A:269:HSI:H51	0.40	2.46	1	1
1:A:238:PRO:O	4:A:269:HSI:H16	0.40	2.17	4	1
1:A:182:ALA:CB	1:A:197:PHE:CD1	0.40	3.04	9	1
1:A:213:PHE:CD1	1:A:214:LEU:N	0.40	2.89	15	1
1:A:175:ASP:OD2	1:A:176:GLY:N	0.40	2.55	2	1
1:A:181:LEU:HD23	1:A:215:THR:CG2	0.40	2.46	2	1
1:A:250:LEU:HD22	1:A:250:LEU:H	0.40	1.76	5	1
1:A:180:ILE:O	1:A:182:ALA:N	0.40	2.54	14	1
1:A:174:PHE:CE2	1:A:180:ILE:HD11	0.40	2.52	1	1
1:A:168:HIS:CE1	1:A:174:PHE:CD2	0.40	3.10	2	1
1:A:161:VAL:HG22	1:A:197:PHE:CE1	0.40	2.52	11	1
1:A:256:ARG:O	1:A:260:SER:CB	0.40	2.69	12	1
1:A:140:VAL:HA	1:A:143:ASN:ND2	0.40	2.32	7	1
1:A:122:THR:HG23	1:A:123:PRO:HD3	0.40	1.92	15	1
1:A:180:ILE:O	1:A:181:LEU:C	0.40	2.60	10	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	147/164 (90%)	111±4 (76±3%)	23±3 (16±2%)	13±4 (9±2%)	2	13
All	All	2205/2460 (90%)	1665 (76%)	350 (16%)	190 (9%)	2	13

All 50 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	167	ALA	9
1	A	248	PHE	8
1	A	180	ILE	8
1	A	173	ALA	8
1	A	207	SER	8
1	A	111	LYS	7
1	A	245	ILE	7
1	A	120	ASN	7
1	A	206	HIS	6
1	A	201	GLU	6
1	A	177	LYS	6
1	A	187	PRO	6
1	A	236	MET	6
1	A	241	LYS	6
1	A	226	LEU	5
1	A	235	VAL	5
1	A	189	SER	5
1	A	119	ASN	5
1	A	121	TYR	4
1	A	208	GLY	4
1	A	227	GLY	4
1	A	122	THR	4
1	A	229	SER	4
1	A	233	LYS	4
1	A	166	GLY	3
1	A	178	GLY	3
1	A	123	PRO	3
1	A	174	PHE	3
1	A	198	ASP	3
1	A	112	HIS	3
1	A	224	LEU	2
1	A	194	ASP	2
1	A	176	GLY	2
1	A	188	GLY	2
1	A	232	PRO	2
1	A	168	HIS	2
1	A	244	ASP	2
1	A	175	ASP	2
1	A	158	ASP	2
1	A	179	GLY	2
1	A	225	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	209	GLY	1
1	A	152	ILE	1
1	A	228	HIS	1
1	A	230	SER	1
1	A	185	PHE	1
1	A	186	GLY	1
1	A	246	ASN	1
1	A	156	MET	1
1	A	190	GLY	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	119/132 (90%)	70±3 (59±3%)	49±3 (41±3%)	0 4
All	All	1785/1980 (90%)	1056 (59%)	729 (41%)	0 4

All 108 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	127	ARG	15
1	A	143	ASN	15
1	A	122	THR	15
1	A	250	LEU	15
1	A	214	LEU	15
1	A	165	ARG	15
1	A	226	LEU	14
1	A	177	LYS	14
1	A	111	LYS	14
1	A	249	ARG	14
1	A	174	PHE	13
1	A	136	LYS	13
1	A	233	LYS	13
1	A	160	LEU	13
1	A	230	SER	12
1	A	259	GLN	12

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Mol	Chain	Res	Type	Models (Total)
1	A	215	THR	12
1	A	197	PHE	11
1	A	118	ILE	11
1	A	114	ILE	10
1	A	200	ASP	10
1	A	117	ARG	10
1	A	147	LEU	10
1	A	175	ASP	10
1	A	236	MET	9
1	A	132	TYR	9
1	A	148	LYS	9
1	A	126	ASN	9
1	A	110	ARG	9
1	A	198	ASP	8
1	A	180	ILE	8
1	A	116	TYR	8
1	A	251	SER	8
1	A	235	VAL	8
1	A	183	HIS	8
1	A	244	ASP	8
1	A	253	ASP	8
1	A	151	LYS	7
1	A	237	PHE	7
1	A	246	ASN	7
1	A	211	ASN	7
1	A	206	HIS	7
1	A	201	GLU	7
1	A	145	THR	7
1	A	223	SER	7
1	A	199	GLU	7
1	A	222	HIS	7
1	A	204	THR	7
1	A	162	VAL	7
1	A	115	THR	7
1	A	163	PHE	6
1	A	191	ILE	6
1	A	189	SER	6
1	A	228	HIS	6
1	A	207	SER	6
1	A	247	THR	6
1	A	239	THR	6
1	A	224	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	202	PHE	6
1	A	219	GLU	6
1	A	154	THR	5
1	A	129	ASP	5
1	A	205	THR	5
1	A	119	ASN	5
1	A	140	VAL	5
1	A	242	TYR	5
1	A	254	ASP	5
1	A	124	ASP	5
1	A	125	MET	5
1	A	161	VAL	5
1	A	231	ASP	5
1	A	194	ASP	5
1	A	185	PHE	4
1	A	135	ARG	4
1	A	229	SER	4
1	A	158	ASP	4
1	A	150	SER	4
1	A	149	PHE	4
1	A	153	ASN	4
1	A	196	HIS	4
1	A	156	MET	4
1	A	212	LEU	4
1	A	258	ILE	4
1	A	139	GLN	4
1	A	240	TYR	4
1	A	134	ILE	3
1	A	112	HIS	3
1	A	120	ASN	3
1	A	121	TYR	3
1	A	241	LYS	3
1	A	210	THR	3
1	A	131	ASP	3
1	A	243	VAL	3
1	A	128	GLU	3
1	A	113	TYR	2
1	A	142	SER	2
1	A	159	ILE	2
1	A	260	SER	2
1	A	203	TRP	2
1	A	181	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	168	HIS	2
1	A	138	PHE	2
1	A	248	PHE	2
1	A	255	ILE	2
1	A	217	VAL	1
1	A	152	ILE	1
1	A	256	ARG	1
1	A	220	ILE	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	HSI	A	269	-	29,29,29	0.75±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	HSI	A	269	-	34,37,37	1.08±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HSI	A	269	-	-	0±0,23,23,23	0±0,2,2,2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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