



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:39 PM UTC

PDB ID : 1Z8R / pdb_00001z8r
Title : 2A cysteine proteinase from human coxsackievirus B4 (strain JVB / Benschoten / New York / 51)
Authors : Baxter, N.J.; Roetzer, A.; Liebig, H.D.; Sedelnikova, S.E.; Hounslow, A.M.; Skern, T.; Waltho, J.P.
Deposited on : 2005-03-31

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

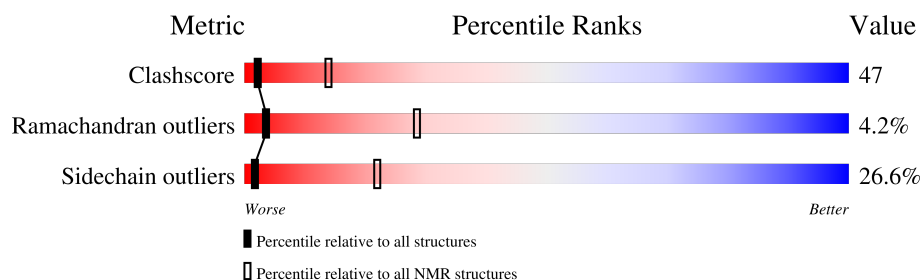
1 Overall quality at a glance

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	166	

2 Ensemble composition and analysis

This entry contains 17 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:9-A:64, A:71-A:103, A:112-A:147 (125)	0.62	7

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

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

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

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2253 atoms, of which 1091 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cocksackievirus B4 polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2252	729	1091	199	225	8	

There are 9 discrepancies between the modelled and reference sequences:

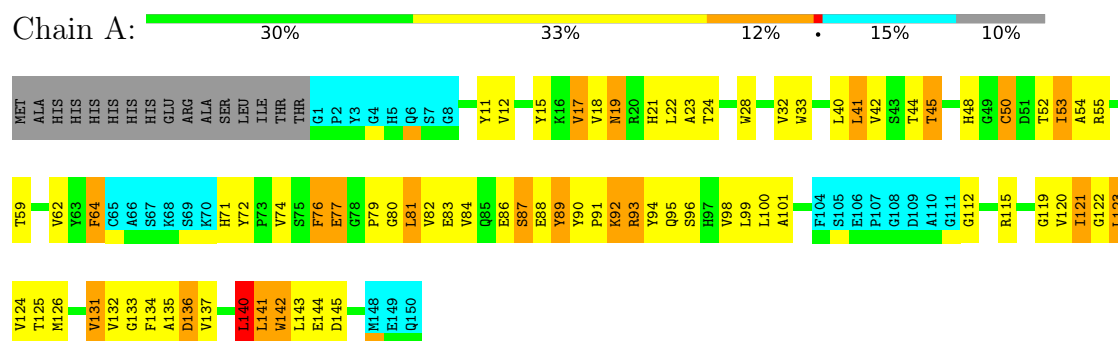
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	cloning artifact	UNP P08292
A	-14	ALA	-	cloning artifact	UNP P08292
A	-13	HIS	-	expression tag	UNP P08292
A	-12	HIS	-	expression tag	UNP P08292
A	-11	HIS	-	expression tag	UNP P08292
A	-10	HIS	-	expression tag	UNP P08292
A	-9	HIS	-	expression tag	UNP P08292
A	-8	HIS	-	expression tag	UNP P08292
A	110	ALA	CYS	engineered mutation	UNP P08292

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4.2.8 Score per residue for model 8

- Molecule 1: Coxsackievirus B4 polyprotein



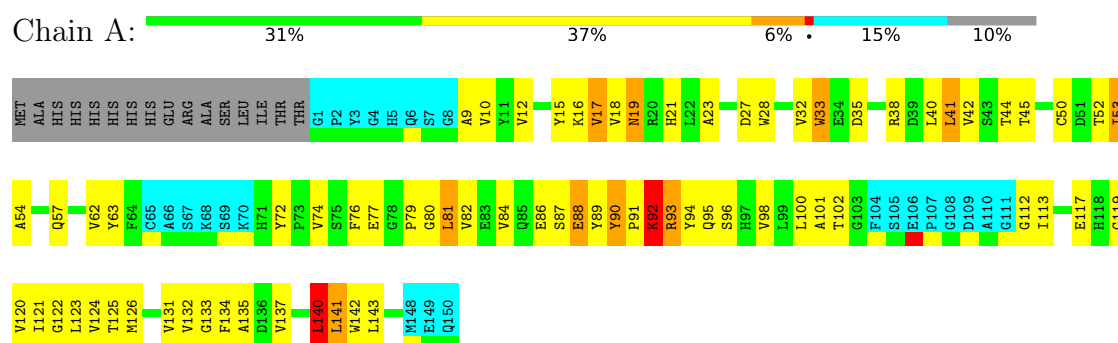
4.2.9 Score per residue for model 9

- Molecule 1: Coxsackievirus B4 polyprotein



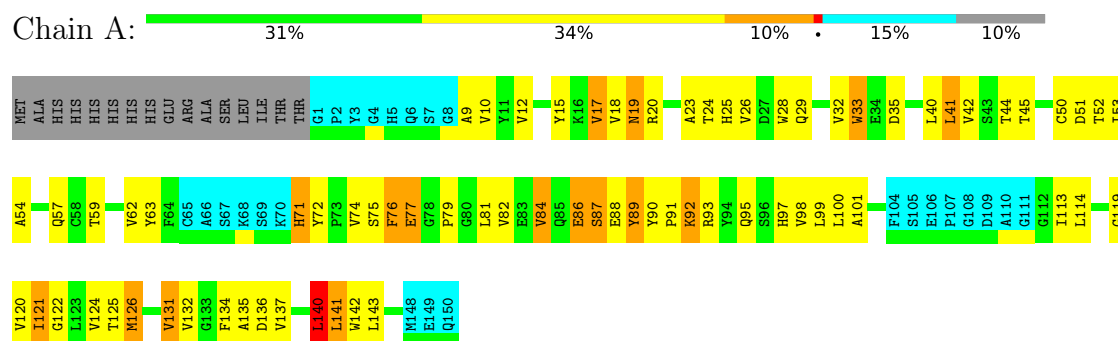
4.2.10 Score per residue for model 10

- Molecule 1: Coxsackievirus B4 polyprotein



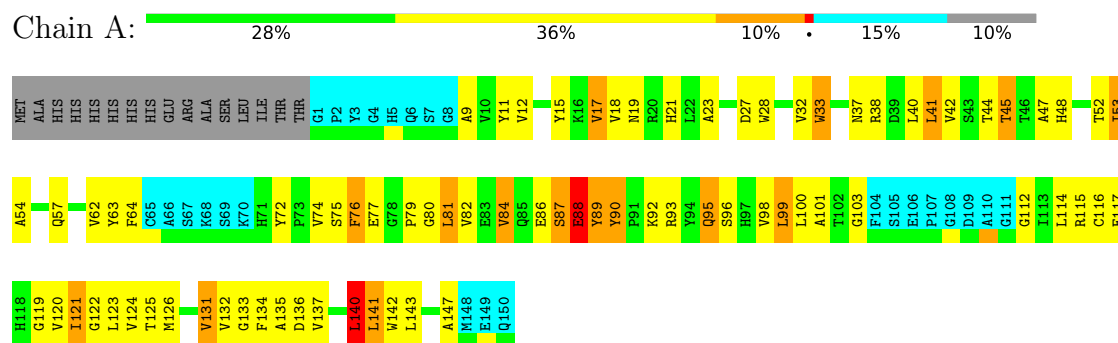
4.2.11 Score per residue for model 11

- Molecule 1: Coxsackievirus B4 polyprotein



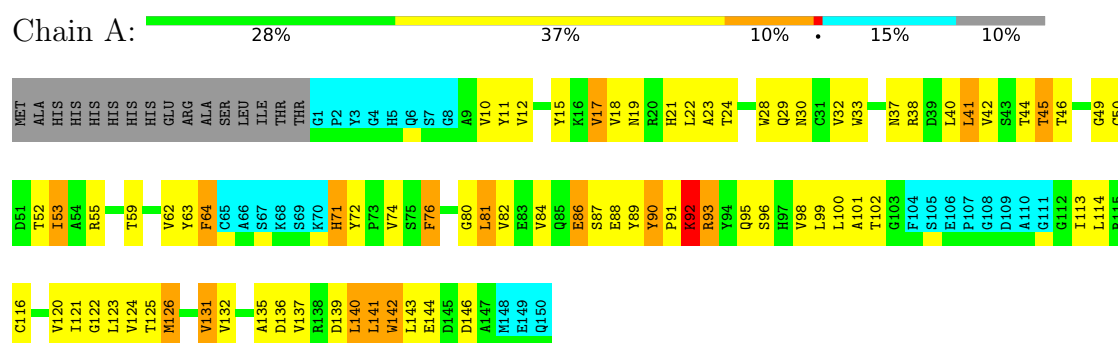
4.2.12 Score per residue for model 12

- Molecule 1: Coxsackievirus B4 polyprotein



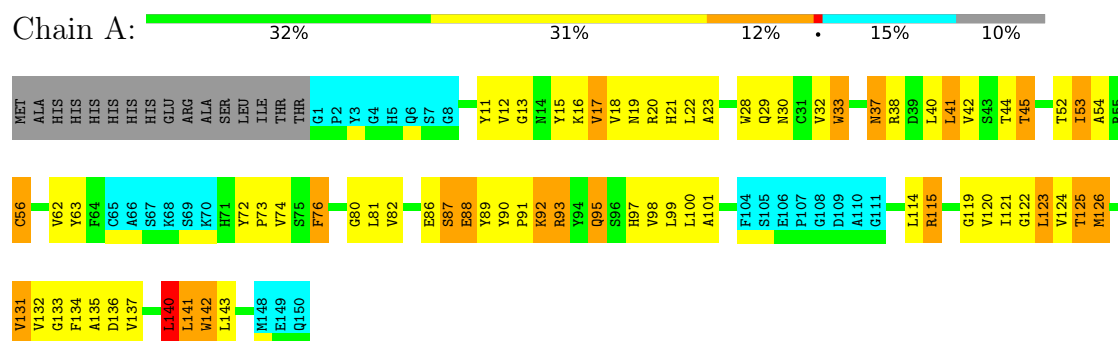
4.2.13 Score per residue for model 13

- Molecule 1: Coxsackievirus B4 polyprotein



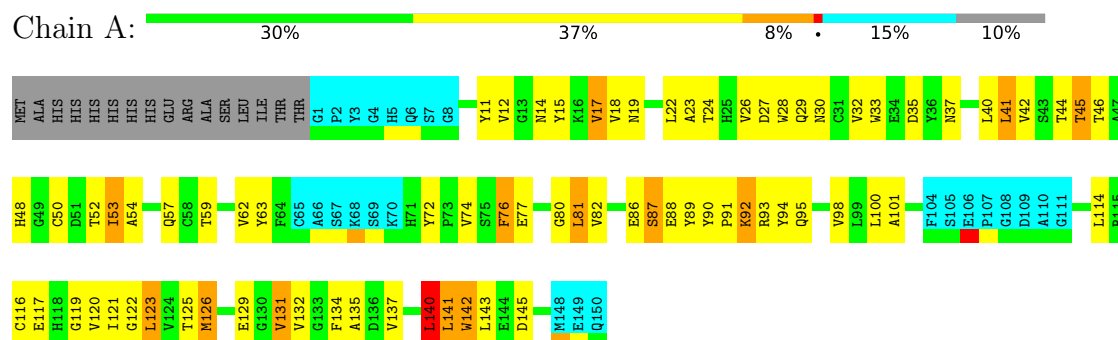
4.2.14 Score per residue for model 14

- Molecule 1: Cocksackievirus B4 polypotein



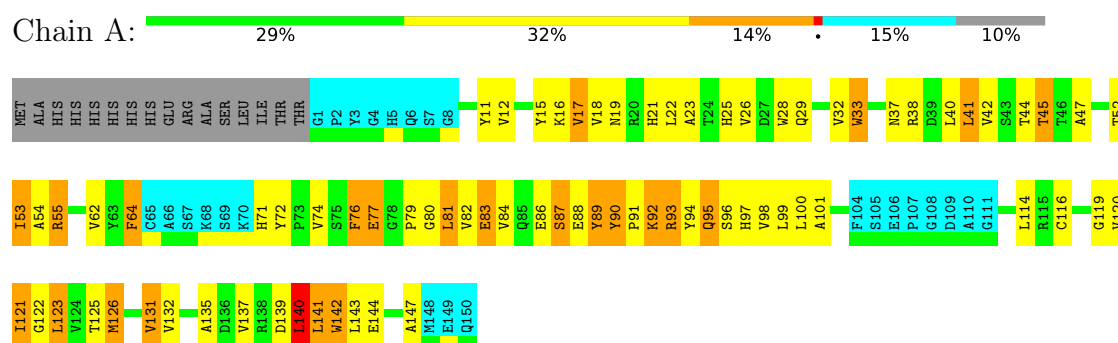
4.2.15 Score per residue for model 15

- Molecule 1: Cocksackievirus B4 polypprotein



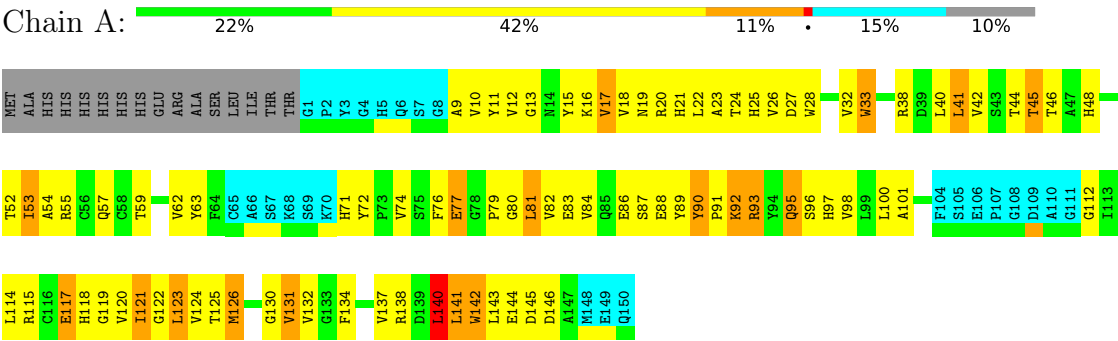
4.2.16 Score per residue for model 16

- Molecule 1: Cocksackievirus B4 polypotein



4.2.17 Score per residue for model 17

- Molecule 1: Coxsackievirus B4 polyprotein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics followed by cartesian slow-cool annealing energy minimisation*.

Of the 100 calculated structures, 17 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	983	932	927	89±5
All	All	16728	15844	15759	1512

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:VAL:HG12	1:A:42:VAL:HG22	0.97	1.36	8	17
1:A:23:ALA:HB3	1:A:28:TRP:CZ2	0.86	2.05	6	8
1:A:84:VAL:HG23	1:A:126:MET:CG	0.84	2.02	11	3
1:A:53:ILE:HB	1:A:141:LEU:HD11	0.84	1.50	13	17
1:A:116:CYS:SG	1:A:121:ILE:HD11	0.83	2.14	13	2
1:A:87:SER:CB	1:A:126:MET:HE1	0.82	2.04	4	4
1:A:11:TYR:CE2	1:A:45:THR:HG21	0.82	2.09	1	10
1:A:116:CYS:HB2	1:A:121:ILE:HD11	0.82	1.52	15	5
1:A:52:THR:O	1:A:120:VAL:HG23	0.81	1.76	17	17
1:A:62:VAL:HG23	1:A:72:TYR:C	0.80	2.01	13	17
1:A:95:GLN:NE2	1:A:125:THR:HG23	0.80	1.92	12	2
1:A:12:VAL:HG21	1:A:53:ILE:HD11	0.79	1.52	8	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:LEU:HD22	1:A:140:LEU:O	0.79	1.78	11	17
1:A:84:VAL:HG23	1:A:126:MET:HG2	0.77	1.55	3	3
1:A:112:GLY:O	1:A:124:VAL:HG23	0.77	1.79	4	2
1:A:42:VAL:HG21	1:A:140:LEU:HD23	0.76	1.54	11	14
1:A:99:LEU:HD11	1:A:136:ASP:HB3	0.75	1.58	12	3
1:A:87:SER:HB2	1:A:126:MET:HE1	0.75	1.57	4	2
1:A:54:ALA:HB2	1:A:119:GLY:N	0.75	1.97	11	15
1:A:9:ALA:HB2	1:A:18:VAL:HG23	0.74	1.56	2	8
1:A:10:VAL:HG22	1:A:113:ILE:HG21	0.74	1.58	13	4
1:A:23:ALA:HB3	1:A:28:TRP:CH2	0.74	2.17	6	8
1:A:87:SER:HB3	1:A:126:MET:HE1	0.74	1.60	8	2
1:A:12:VAL:HG13	1:A:144:GLU:OE2	0.73	1.83	16	1
1:A:40:LEU:HD13	1:A:123:LEU:HD11	0.73	1.59	16	6
1:A:100:LEU:HA	1:A:132:VAL:O	0.72	1.84	1	15
1:A:90:TYR:HB3	1:A:126:MET:HE3	0.72	1.59	15	1
1:A:122:GLY:HA2	1:A:137:VAL:HG23	0.72	1.60	12	17
1:A:125:THR:OG1	1:A:135:ALA:HB2	0.72	1.85	1	15
1:A:100:LEU:HD23	1:A:132:VAL:C	0.72	2.10	1	17
1:A:54:ALA:HB1	1:A:56:CYS:SG	0.71	2.24	14	2
1:A:19:ASN:HB2	1:A:22:LEU:HD12	0.70	1.64	7	1
1:A:100:LEU:HD23	1:A:132:VAL:O	0.70	1.87	13	16
1:A:76:PHE:CZ	1:A:114:LEU:HD21	0.70	2.22	2	6
1:A:10:VAL:HB	1:A:113:ILE:HG21	0.69	1.63	10	3
1:A:112:GLY:O	1:A:124:VAL:HG13	0.69	1.87	17	4
1:A:123:LEU:CD1	1:A:135:ALA:HB3	0.69	2.16	14	1
1:A:84:VAL:HG23	1:A:126:MET:HG3	0.69	1.62	4	3
1:A:18:VAL:O	1:A:40:LEU:HD12	0.69	1.86	10	14
1:A:63:TYR:CZ	1:A:132:VAL:HG11	0.69	2.22	15	3
1:A:54:ALA:HB2	1:A:119:GLY:CA	0.69	2.18	6	12
1:A:84:VAL:HG13	1:A:126:MET:CG	0.68	2.18	13	2
1:A:17:VAL:HG23	1:A:40:LEU:HD11	0.68	1.65	1	15
1:A:95:GLN:OE1	1:A:125:THR:HG23	0.68	1.87	7	1
1:A:141:LEU:C	1:A:143:LEU:HD12	0.68	2.14	13	16
1:A:123:LEU:CD2	1:A:135:ALA:HB3	0.67	2.20	3	1
1:A:28:TRP:NE1	1:A:41:LEU:HD12	0.67	2.05	17	8
1:A:84:VAL:HG22	1:A:126:MET:HB2	0.66	1.67	12	1
1:A:99:LEU:HD11	1:A:136:ASP:OD2	0.65	1.91	8	3
1:A:23:ALA:HB3	1:A:28:TRP:NE1	0.65	2.07	10	9
1:A:123:LEU:HD13	1:A:123:LEU:N	0.65	2.06	3	1
1:A:84:VAL:HG13	1:A:126:MET:HG2	0.65	1.68	17	3
1:A:33:TRP:CE3	1:A:42:VAL:HG23	0.65	2.26	8	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:GLU:C	1:A:79:PRO:HD3	0.65	2.17	6	7
1:A:54:ALA:O	1:A:147:ALA:HB3	0.64	1.91	3	1
1:A:62:VAL:HG21	1:A:71:HIS:HB2	0.64	1.69	8	4
1:A:76:PHE:CD2	1:A:101:ALA:HB2	0.64	2.27	5	11
1:A:63:TYR:OH	1:A:132:VAL:HG11	0.64	1.92	15	2
1:A:41:LEU:HD23	1:A:41:LEU:O	0.63	1.92	4	17
1:A:125:THR:HG22	1:A:126:MET:N	0.63	2.09	10	15
1:A:24:THR:HG23	1:A:26:VAL:HG12	0.63	1.71	15	4
1:A:84:VAL:HG23	1:A:126:MET:HB2	0.63	1.69	16	1
1:A:87:SER:O	1:A:126:MET:HE1	0.62	1.94	12	1
1:A:76:PHE:CZ	1:A:114:LEU:HD11	0.62	2.29	14	9
1:A:11:TYR:OH	1:A:47:ALA:HB3	0.62	1.93	12	2
1:A:42:VAL:CG2	1:A:140:LEU:HD23	0.62	2.24	11	15
1:A:25:HIS:CE1	1:A:26:VAL:HG23	0.62	2.30	16	1
1:A:99:LEU:HD11	1:A:136:ASP:HB2	0.62	1.70	14	2
1:A:63:TYR:CE2	1:A:74:VAL:HG21	0.62	2.30	13	9
1:A:116:CYS:CB	1:A:121:ILE:HD11	0.62	2.25	1	2
1:A:101:ALA:O	1:A:132:VAL:HG23	0.61	1.94	2	3
1:A:137:VAL:HG12	1:A:137:VAL:O	0.61	1.96	7	16
1:A:11:TYR:CE1	1:A:45:THR:HG21	0.61	2.30	17	1
1:A:123:LEU:C	1:A:123:LEU:HD22	0.60	2.21	14	1
1:A:81:LEU:HD11	1:A:94:TYR:HB3	0.60	1.72	1	6
1:A:81:LEU:HD22	1:A:96:SER:HB2	0.60	1.72	6	5
1:A:121:ILE:HD12	1:A:121:ILE:N	0.60	2.12	2	4
1:A:116:CYS:HB2	1:A:121:ILE:HD12	0.60	1.71	12	1
1:A:11:TYR:CZ	1:A:45:THR:HG21	0.59	2.32	1	2
1:A:18:VAL:C	1:A:40:LEU:HD12	0.59	2.22	8	12
1:A:9:ALA:HB2	1:A:18:VAL:CG2	0.59	2.27	2	3
1:A:23:ALA:HB2	1:A:41:LEU:HD21	0.59	1.75	8	2
1:A:32:VAL:CG2	1:A:42:VAL:HG12	0.59	2.28	12	13
1:A:52:THR:HG23	1:A:144:GLU:OE2	0.59	1.97	17	1
1:A:140:LEU:O	1:A:143:LEU:HD11	0.59	1.98	8	12
1:A:33:TRP:CZ3	1:A:42:VAL:HG23	0.59	2.33	13	10
1:A:33:TRP:CH2	1:A:40:LEU:HD23	0.58	2.33	2	5
1:A:140:LEU:CD1	1:A:140:LEU:N	0.58	2.66	10	17
1:A:37:ASN:O	1:A:95:GLN:HA	0.58	1.98	9	8
1:A:88:GLU:O	1:A:89:TYR:CD1	0.58	2.56	12	1
1:A:141:LEU:HD12	1:A:146:ASP:OD1	0.58	1.98	17	1
1:A:74:VAL:CG1	1:A:101:ALA:HB1	0.58	2.29	1	7
1:A:86:GLU:HA	1:A:90:TYR:O	0.58	1.97	3	16
1:A:52:THR:C	1:A:120:VAL:HG23	0.57	2.25	3	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:N	1:A:41:LEU:CD2	0.57	2.68	8	2
1:A:15:TYR:HB2	1:A:143:LEU:HD23	0.57	1.75	11	14
1:A:15:TYR:CB	1:A:143:LEU:HD23	0.57	2.30	1	16
1:A:76:PHE:CE2	1:A:114:LEU:HD21	0.57	2.35	1	3
1:A:100:LEU:HD22	1:A:131:VAL:CG1	0.57	2.29	17	14
1:A:12:VAL:HG21	1:A:53:ILE:CD1	0.57	2.29	3	5
1:A:33:TRP:HH2	1:A:40:LEU:HD23	0.56	1.61	8	8
1:A:141:LEU:O	1:A:143:LEU:N	0.56	2.37	13	17
1:A:23:ALA:CB	1:A:41:LEU:HD11	0.56	2.30	5	7
1:A:132:VAL:HG11	1:A:134:PHE:CZ	0.56	2.36	5	2
1:A:17:VAL:CG1	1:A:42:VAL:HG22	0.56	2.23	15	10
1:A:41:LEU:HD23	1:A:41:LEU:C	0.55	2.27	1	15
1:A:63:TYR:HE2	1:A:74:VAL:HG21	0.55	1.61	9	7
1:A:76:PHE:HD2	1:A:101:ALA:HB2	0.55	1.61	11	4
1:A:28:TRP:HE1	1:A:41:LEU:HD12	0.55	1.61	17	7
1:A:79:PRO:HD2	1:A:98:VAL:O	0.55	2.01	11	7
1:A:76:PHE:HZ	1:A:114:LEU:HD11	0.55	1.62	13	2
1:A:53:ILE:CG2	1:A:141:LEU:HD11	0.55	2.31	11	1
1:A:137:VAL:O	1:A:141:LEU:HD22	0.55	2.01	9	8
1:A:38:ARG:CZ	1:A:40:LEU:HD22	0.55	2.32	9	1
1:A:99:LEU:HD13	1:A:136:ASP:CG	0.54	2.27	4	1
1:A:23:ALA:HB3	1:A:28:TRP:HE1	0.54	1.61	10	9
1:A:137:VAL:O	1:A:137:VAL:HG12	0.54	2.01	9	1
1:A:99:LEU:HD12	1:A:134:PHE:O	0.54	2.03	12	1
1:A:15:TYR:CE1	1:A:44:THR:HG22	0.54	2.37	4	17
1:A:84:VAL:HG21	1:A:90:TYR:CD1	0.54	2.38	3	1
1:A:25:HIS:CD2	1:A:26:VAL:HG23	0.54	2.37	17	1
1:A:19:ASN:ND2	1:A:123:LEU:HD12	0.54	2.18	15	1
1:A:132:VAL:O	1:A:132:VAL:HG23	0.53	2.02	8	12
1:A:124:VAL:O	1:A:124:VAL:HG13	0.53	2.04	1	5
1:A:95:GLN:CD	1:A:125:THR:HG21	0.53	2.29	13	1
1:A:41:LEU:C	1:A:41:LEU:CD2	0.53	2.82	17	15
1:A:87:SER:O	1:A:89:TYR:N	0.53	2.41	16	16
1:A:123:LEU:N	1:A:123:LEU:HD23	0.53	2.18	16	5
1:A:12:VAL:HB	1:A:143:LEU:HD22	0.53	1.81	4	7
1:A:10:VAL:HG13	1:A:10:VAL:O	0.53	2.03	3	5
1:A:28:TRP:CZ2	1:A:41:LEU:CD1	0.53	2.92	8	6
1:A:12:VAL:HG21	1:A:53:ILE:HG12	0.53	1.81	11	1
1:A:84:VAL:HG22	1:A:93:ARG:O	0.52	2.03	9	2
1:A:84:VAL:HG11	1:A:95:GLN:OE1	0.52	2.05	6	1
1:A:40:LEU:HD13	1:A:123:LEU:HD21	0.52	1.80	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:HD11	1:A:136:ASP:CB	0.52	2.35	14	2
1:A:115:ARG:HD3	1:A:120:VAL:HG22	0.52	1.80	6	2
1:A:84:VAL:HG12	1:A:93:ARG:O	0.52	2.05	8	4
1:A:40:LEU:HD13	1:A:123:LEU:CD1	0.52	2.34	7	2
1:A:17:VAL:HG12	1:A:42:VAL:CG2	0.52	2.25	14	5
1:A:24:THR:CG2	1:A:26:VAL:HG12	0.52	2.34	15	4
1:A:74:VAL:CG1	1:A:76:PHE:CE2	0.52	2.92	8	7
1:A:53:ILE:HD12	1:A:137:VAL:HG11	0.52	1.80	7	6
1:A:82:VAL:HB	1:A:98:VAL:HG11	0.52	1.82	6	16
1:A:41:LEU:O	1:A:41:LEU:CD2	0.51	2.58	9	15
1:A:81:LEU:HD22	1:A:96:SER:HB3	0.51	1.80	3	4
1:A:123:LEU:HD11	1:A:135:ALA:HB3	0.51	1.81	14	1
1:A:101:ALA:O	1:A:132:VAL:N	0.51	2.43	5	13
1:A:12:VAL:CG2	1:A:53:ILE:HD11	0.51	2.33	3	2
1:A:53:ILE:CB	1:A:141:LEU:HD11	0.51	2.34	14	13
1:A:23:ALA:O	1:A:28:TRP:CZ3	0.51	2.64	1	8
1:A:10:VAL:HG13	1:A:17:VAL:HG22	0.51	1.82	2	3
1:A:141:LEU:O	1:A:143:LEU:HD12	0.51	2.06	5	5
1:A:121:ILE:HG22	1:A:136:ASP:OD1	0.51	2.06	8	2
1:A:114:LEU:HD22	1:A:134:PHE:HD2	0.51	1.66	15	4
1:A:32:VAL:HG22	1:A:42:VAL:O	0.50	2.05	10	14
1:A:76:PHE:CD1	1:A:76:PHE:N	0.50	2.79	6	14
1:A:99:LEU:HD21	1:A:136:ASP:OD2	0.50	2.06	1	1
1:A:10:VAL:CG2	1:A:113:ILE:HG21	0.50	2.36	13	3
1:A:123:LEU:HD22	1:A:135:ALA:HB3	0.50	1.84	3	1
1:A:126:MET:O	1:A:133:GLY:HA3	0.50	2.07	8	7
1:A:41:LEU:N	1:A:41:LEU:HD22	0.50	2.21	7	1
1:A:38:ARG:NH2	1:A:40:LEU:HD22	0.50	2.22	12	1
1:A:101:ALA:O	1:A:131:VAL:HG12	0.49	2.07	7	1
1:A:62:VAL:HG23	1:A:72:TYR:O	0.49	2.07	13	1
1:A:12:VAL:HG21	1:A:53:ILE:CG1	0.49	2.37	11	1
1:A:76:PHE:CE1	1:A:114:LEU:HD21	0.49	2.42	12	2
1:A:15:TYR:HE1	1:A:44:THR:HG22	0.49	1.68	8	17
1:A:142:TRP:C	1:A:143:LEU:HD12	0.49	2.33	1	7
1:A:24:THR:HG23	1:A:26:VAL:CG1	0.49	2.37	15	3
1:A:84:VAL:HG21	1:A:90:TYR:HD2	0.49	1.67	16	1
1:A:140:LEU:O	1:A:140:LEU:CD2	0.49	2.57	11	9
1:A:18:VAL:O	1:A:41:LEU:CD2	0.49	2.60	8	2
1:A:24:THR:OG1	1:A:26:VAL:HG12	0.49	2.06	5	1
1:A:132:VAL:CG1	1:A:134:PHE:CE2	0.49	2.96	2	4
1:A:132:VAL:HB	1:A:134:PHE:CZ	0.49	2.42	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ALA:HA	1:A:147:ALA:HB3	0.49	1.84	12	3
1:A:62:VAL:HG21	1:A:71:HIS:HB3	0.49	1.85	17	3
1:A:81:LEU:HD22	1:A:96:SER:CB	0.49	2.38	7	5
1:A:95:GLN:HE22	1:A:125:THR:HG23	0.49	1.68	4	1
1:A:138:ARG:HA	1:A:141:LEU:HD23	0.48	1.85	4	2
1:A:46:THR:O	1:A:46:THR:HG23	0.48	2.08	4	1
1:A:112:GLY:O	1:A:124:VAL:HG22	0.48	2.08	6	1
1:A:28:TRP:CE2	1:A:41:LEU:HD11	0.48	2.44	8	1
1:A:84:VAL:O	1:A:92:LYS:HA	0.48	2.09	7	8
1:A:63:TYR:CD1	1:A:63:TYR:C	0.48	2.91	1	9
1:A:124:VAL:HG22	1:A:134:PHE:HE1	0.48	1.68	5	1
1:A:87:SER:HB3	1:A:126:MET:HE2	0.48	1.86	6	1
1:A:59:THR:HG22	1:A:76:PHE:O	0.48	2.09	13	1
1:A:74:VAL:HG11	1:A:101:ALA:HB1	0.48	1.86	1	4
1:A:63:TYR:CD1	1:A:63:TYR:O	0.48	2.66	3	5
1:A:10:VAL:HG22	1:A:113:ILE:CG2	0.48	2.36	13	1
1:A:99:LEU:HD11	1:A:136:ASP:CG	0.48	2.33	11	2
1:A:137:VAL:O	1:A:137:VAL:CG1	0.48	2.62	17	8
1:A:132:VAL:CG2	1:A:134:PHE:CZ	0.47	2.97	8	5
1:A:63:TYR:CG	1:A:134:PHE:CZ	0.47	3.02	15	1
1:A:99:LEU:HD12	1:A:99:LEU:N	0.47	2.24	16	2
1:A:126:MET:HA	1:A:126:MET:HE2	0.47	1.87	17	1
1:A:23:ALA:O	1:A:28:TRP:CH2	0.47	2.68	7	7
1:A:91:PRO:O	1:A:93:ARG:N	0.47	2.47	9	12
1:A:132:VAL:CG1	1:A:134:PHE:CZ	0.47	2.97	1	3
1:A:137:VAL:O	1:A:140:LEU:HD13	0.47	2.09	2	4
1:A:18:VAL:O	1:A:41:LEU:HD22	0.47	2.10	4	12
1:A:123:LEU:N	1:A:123:LEU:CD1	0.47	2.77	3	1
1:A:74:VAL:CG1	1:A:101:ALA:CB	0.47	2.93	10	6
1:A:28:TRP:CE2	1:A:41:LEU:CD1	0.47	2.98	8	1
1:A:63:TYR:CE2	1:A:74:VAL:CG2	0.47	2.98	13	1
1:A:84:VAL:HG23	1:A:126:MET:CB	0.47	2.39	8	1
1:A:90:TYR:HB2	1:A:126:MET:HE3	0.46	1.87	4	1
1:A:10:VAL:HG23	1:A:51:ASP:OD2	0.46	2.11	2	1
1:A:18:VAL:HG22	1:A:19:ASN:N	0.46	2.25	1	17
1:A:100:LEU:HD22	1:A:131:VAL:HG12	0.46	1.86	17	3
1:A:11:TYR:HE2	1:A:45:THR:HG21	0.46	1.66	4	2
1:A:11:TYR:CE1	1:A:49:GLY:CA	0.46	2.99	13	1
1:A:115:ARG:CD	1:A:120:VAL:HG22	0.46	2.41	6	1
1:A:76:PHE:CE2	1:A:114:LEU:CD2	0.46	2.99	11	2
1:A:76:PHE:HB3	1:A:101:ALA:HB2	0.46	1.86	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:HD22	1:A:131:VAL:HB	0.46	1.88	5	2
1:A:122:GLY:HA3	1:A:135:ALA:O	0.46	2.11	16	4
1:A:17:VAL:CG2	1:A:40:LEU:HD21	0.46	2.40	8	1
1:A:63:TYR:CZ	1:A:72:TYR:CB	0.46	2.98	5	3
1:A:15:TYR:CE2	1:A:142:TRP:CE3	0.45	3.04	7	12
1:A:76:PHE:CZ	1:A:114:LEU:CD2	0.45	2.99	12	1
1:A:115:ARG:HD3	1:A:120:VAL:HG13	0.45	1.87	6	1
1:A:61:GLY:N	1:A:76:PHE:CE1	0.45	2.84	4	2
1:A:125:THR:CG2	1:A:126:MET:N	0.45	2.79	14	4
1:A:62:VAL:HG12	1:A:115:ARG:O	0.45	2.10	14	1
1:A:9:ALA:CB	1:A:18:VAL:HG23	0.45	2.34	2	1
1:A:17:VAL:HA	1:A:41:LEU:O	0.45	2.12	16	9
1:A:54:ALA:HB2	1:A:119:GLY:C	0.45	2.37	3	1
1:A:77:GLU:O	1:A:79:PRO:HD3	0.45	2.12	5	4
1:A:24:THR:O	1:A:28:TRP:HD1	0.45	1.95	13	2
1:A:11:TYR:CE1	1:A:13:GLY:O	0.45	2.70	17	4
1:A:24:THR:O	1:A:28:TRP:CE3	0.45	2.70	7	4
1:A:114:LEU:HD22	1:A:134:PHE:CD2	0.44	2.46	15	3
1:A:116:CYS:N	1:A:121:ILE:CD1	0.44	2.80	1	2
1:A:132:VAL:O	1:A:132:VAL:CG2	0.44	2.65	10	9
1:A:84:VAL:HG23	1:A:126:MET:SD	0.44	2.53	6	1
1:A:81:LEU:HD13	1:A:95:GLN:O	0.44	2.13	1	2
1:A:11:TYR:C	1:A:11:TYR:CD1	0.44	2.96	6	7
1:A:76:PHE:CZ	1:A:114:LEU:CD1	0.44	3.00	7	3
1:A:38:ARG:NE	1:A:38:ARG:HA	0.44	2.27	10	1
1:A:123:LEU:HD13	1:A:135:ALA:HB3	0.44	1.88	14	1
1:A:11:TYR:CE1	1:A:45:THR:CG2	0.44	2.99	17	1
1:A:10:VAL:HG21	1:A:120:VAL:HG11	0.44	1.90	3	1
1:A:82:VAL:CG2	1:A:98:VAL:CG1	0.44	2.95	17	15
1:A:76:PHE:CB	1:A:101:ALA:HB2	0.44	2.43	6	3
1:A:61:GLY:O	1:A:73:PRO:HA	0.44	2.12	6	1
1:A:28:TRP:NE1	1:A:41:LEU:CD1	0.44	2.80	7	1
1:A:37:ASN:O	1:A:94:TYR:O	0.44	2.36	9	1
1:A:11:TYR:CE2	1:A:45:THR:CG2	0.44	2.98	13	1
1:A:140:LEU:O	1:A:143:LEU:CD1	0.43	2.66	7	8
1:A:123:LEU:HD22	1:A:123:LEU:H	0.43	1.73	3	1
1:A:38:ARG:CZ	1:A:40:LEU:CD2	0.43	2.96	9	1
1:A:38:ARG:NH1	1:A:96:SER:O	0.43	2.52	10	1
1:A:112:GLY:C	1:A:124:VAL:HG23	0.43	2.38	4	1
1:A:23:ALA:HB2	1:A:41:LEU:HD11	0.43	1.88	5	2
1:A:121:ILE:N	1:A:121:ILE:CD1	0.43	2.81	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TRP:CZ2	1:A:41:LEU:HD12	0.43	2.49	3	2
1:A:77:GLU:O	1:A:99:LEU:HA	0.43	2.13	5	1
1:A:11:TYR:CD1	1:A:11:TYR:C	0.43	2.96	7	2
1:A:79:PRO:HD2	1:A:99:LEU:HA	0.43	1.90	12	1
1:A:84:VAL:HG12	1:A:126:MET:CG	0.43	2.43	9	1
1:A:25:HIS:CE1	1:A:26:VAL:CG2	0.43	3.00	16	1
1:A:132:VAL:HG11	1:A:134:PHE:CE2	0.43	2.49	11	2
1:A:77:GLU:O	1:A:79:PRO:CD	0.43	2.66	12	5
1:A:74:VAL:HG12	1:A:76:PHE:CE2	0.43	2.48	8	1
1:A:62:VAL:HG23	1:A:73:PRO:N	0.43	2.27	14	1
1:A:55:ARG:H	1:A:147:ALA:HB3	0.43	1.74	5	3
1:A:15:TYR:HB3	1:A:143:LEU:HD23	0.43	1.89	8	2
1:A:57:GLN:O	1:A:58:CYS:O	0.43	2.37	9	1
1:A:53:ILE:HA	1:A:120:VAL:HB	0.42	1.91	13	3
1:A:20:ARG:CD	1:A:21:HIS:N	0.42	2.81	4	1
1:A:12:VAL:HG11	1:A:143:LEU:HB2	0.42	1.90	8	1
1:A:140:LEU:N	1:A:140:LEU:HD12	0.42	2.29	12	2
1:A:33:TRP:CZ2	1:A:35:ASP:OD1	0.42	2.72	10	1
1:A:17:VAL:O	1:A:17:VAL:CG2	0.42	2.68	12	9
1:A:95:GLN:OE1	1:A:125:THR:HG21	0.42	2.14	13	1
1:A:95:GLN:CD	1:A:125:THR:HG23	0.42	2.39	12	1
1:A:38:ARG:O	1:A:38:ARG:NE	0.42	2.52	2	1
1:A:77:GLU:O	1:A:79:PRO:HD2	0.42	2.15	10	4
1:A:117:GLU:CG	1:A:118:HIS:CE1	0.42	3.03	4	1
1:A:12:VAL:CG1	1:A:144:GLU:HB2	0.42	2.45	2	1
1:A:11:TYR:CD1	1:A:45:THR:HG21	0.42	2.48	17	1
1:A:14:ASN:O	1:A:44:THR:HA	0.42	2.15	15	1
1:A:114:LEU:HG	1:A:121:ILE:HB	0.42	1.91	17	1
1:A:64:PHE:CB	1:A:71:HIS:CD2	0.42	3.03	3	1
1:A:95:GLN:NE2	1:A:125:THR:HG21	0.42	2.29	13	1
1:A:84:VAL:O	1:A:84:VAL:HG12	0.41	2.14	12	1
1:A:125:THR:OG1	1:A:135:ALA:CB	0.41	2.67	13	1
1:A:84:VAL:HB	1:A:126:MET:CG	0.41	2.45	9	1
1:A:15:TYR:CE2	1:A:142:TRP:CZ3	0.41	3.08	13	1
1:A:63:TYR:HB2	1:A:134:PHE:CZ	0.41	2.50	1	1
1:A:28:TRP:CH2	1:A:41:LEU:HD12	0.41	2.50	3	1
1:A:38:ARG:NE	1:A:135:ALA:CB	0.41	2.83	16	1
1:A:17:VAL:CG2	1:A:40:LEU:HD11	0.41	2.43	2	1
1:A:81:LEU:HD22	1:A:96:SER:HA	0.41	1.91	9	1
1:A:82:VAL:HB	1:A:98:VAL:CG1	0.41	2.46	9	2
1:A:140:LEU:N	1:A:140:LEU:HD13	0.41	2.30	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:HD2	1:A:135:ALA:HB1	0.41	1.92	13	1
1:A:27:ASP:O	1:A:31:CYS:HB2	0.41	2.16	7	1
1:A:38:ARG:NH2	1:A:95:GLN:NE2	0.41	2.68	17	1
1:A:84:VAL:CG1	1:A:126:MET:CG	0.41	2.98	9	1
1:A:17:VAL:CG2	1:A:17:VAL:O	0.41	2.69	2	1
1:A:23:ALA:CB	1:A:28:TRP:NE1	0.41	2.84	11	2
1:A:21:HIS:CD2	1:A:90:TYR:CE1	0.41	3.09	10	1
1:A:12:VAL:HG22	1:A:51:ASP:O	0.41	2.15	11	1
1:A:112:GLY:O	1:A:124:VAL:HG12	0.41	2.15	12	1
1:A:12:VAL:HG13	1:A:144:GLU:CD	0.41	2.38	16	1
1:A:83:GLU:OE2	1:A:94:TYR:CE1	0.41	2.74	16	1
1:A:83:GLU:OE1	1:A:94:TYR:CZ	0.41	2.74	16	1
1:A:63:TYR:CE1	1:A:72:TYR:HB2	0.41	2.51	5	1
1:A:84:VAL:HG11	1:A:95:GLN:CD	0.41	2.41	16	1
1:A:123:LEU:HD22	1:A:124:VAL:O	0.40	2.16	14	1
1:A:101:ALA:O	1:A:131:VAL:HA	0.40	2.17	16	1
1:A:36:TYR:CE2	1:A:37:ASN:OD1	0.40	2.75	1	1
1:A:38:ARG:NE	1:A:135:ALA:HB1	0.40	2.30	16	1
1:A:40:LEU:CD1	1:A:123:LEU:HD11	0.40	2.46	2	1
1:A:83:GLU:CD	1:A:94:TYR:CE1	0.40	3.00	3	1
1:A:28:TRP:CZ2	1:A:41:LEU:HD11	0.40	2.51	8	1
1:A:132:VAL:HB	1:A:134:PHE:CE1	0.40	2.51	8	1
1:A:132:VAL:CG2	1:A:134:PHE:CE2	0.40	3.05	14	1
1:A:83:GLU:OE1	1:A:94:TYR:CE1	0.40	2.75	16	1
1:A:117:GLU:CD	1:A:118:HIS:CE1	0.40	3.00	17	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	125/166 (75%)	108±1 (87±1%)	11±1 (9±1%)	5±1 (4±1%)	3	28
All	All	2125/2822 (75%)	1840 (87%)	195 (9%)	90 (4%)	3	28

All 13 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	88	GLU	17
1	A	142	TRP	17
1	A	80	GLY	15
1	A	92	LYS	15
1	A	140	LEU	14
1	A	64	PHE	3
1	A	50	CYS	2
1	A	130	GLY	2
1	A	112	GLY	1
1	A	9	ALA	1
1	A	58	CYS	1
1	A	89	TYR	1
1	A	103	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	105/137 (77%)	77±4 (73±3%)	28±4 (27±3%)	2	22
All	All	1785/2329 (77%)	1311 (73%)	474 (27%)	2	22

All 67 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	17	VAL	17
1	A	41	LEU	17
1	A	45	THR	17
1	A	76	PHE	17
1	A	81	LEU	17
1	A	131	VAL	17
1	A	140	LEU	17
1	A	141	LEU	17
1	A	92	LYS	16
1	A	53	ILE	15
1	A	123	LEU	14
1	A	121	ILE	12
1	A	87	SER	11

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Mol	Chain	Res	Type	Models (Total)
1	A	126	MET	11
1	A	33	TRP	11
1	A	93	ARG	10
1	A	21	HIS	10
1	A	22	LEU	10
1	A	16	LYS	9
1	A	27	ASP	9
1	A	50	CYS	9
1	A	57	GLN	9
1	A	97	HIS	9
1	A	95	GLN	9
1	A	55	ARG	8
1	A	59	THR	8
1	A	83	GLU	7
1	A	144	GLU	7
1	A	77	GLU	7
1	A	115	ARG	7
1	A	29	GLN	7
1	A	20	ARG	6
1	A	88	GLU	6
1	A	30	ASN	6
1	A	64	PHE	6
1	A	90	TYR	6
1	A	46	THR	5
1	A	71	HIS	5
1	A	48	HIS	5
1	A	39	ASP	4
1	A	145	ASP	4
1	A	75	SER	4
1	A	138	ARG	4
1	A	19	ASN	4
1	A	117	GLU	4
1	A	34	GLU	3
1	A	86	GLU	3
1	A	84	VAL	3
1	A	129	GLU	3
1	A	38	ARG	3
1	A	37	ASN	3
1	A	89	TYR	3
1	A	125	THR	3
1	A	85	GLN	2
1	A	132	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	24	THR	2
1	A	102	THR	2
1	A	35	ASP	2
1	A	139	ASP	2
1	A	96	SER	1
1	A	60	THR	1
1	A	14	ASN	1
1	A	136	ASP	1
1	A	25	HIS	1
1	A	99	LEU	1
1	A	146	ASP	1
1	A	56	CYS	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided