



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 05:16 AM UTC

PDB ID : 1CRR / pdb_00001crr
Title : THE SOLUTION STRUCTURE AND DYNAMICS OF RAS P21. GDP DETERMINED BY HETERONUCLEAR THREE AND FOUR DIMENSIONAL NMR SPECTROSCOPY
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Deposited on : 1993-11-24

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

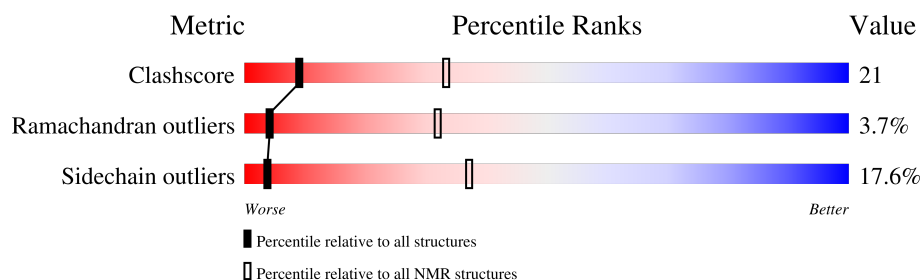
1 Overall quality at a glance

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	54% 39% • 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 37 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:1-A:59, A:67-A:119, A:123-A:166 (156)	0.76	37

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 5 single-model clusters were found.

Cluster number	Models
1	22, 24, 25, 26, 27, 36, 37, 38, 39
2	32, 40
3	23, 30
4	31, 33
Single-model clusters	21; 28; 29; 34; 35

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2672 atoms, of which 1316 are hydrogens and 0 are deuteriums.

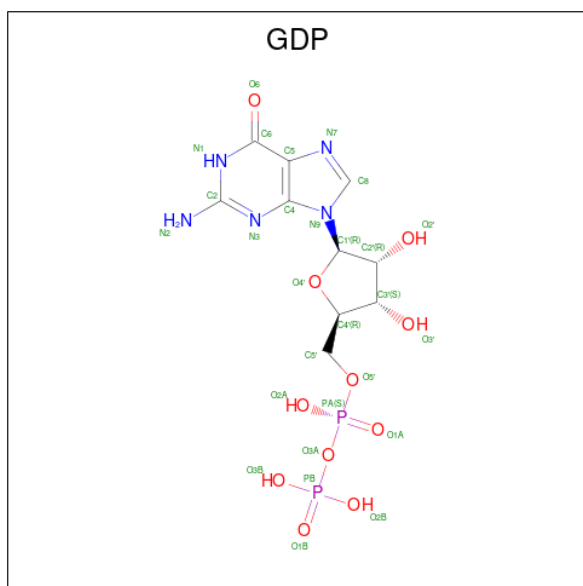
- Molecule 1 is a protein called C-H-RAS P21 PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2619	824	1296	228	264	7	

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Mg
			1	1

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: C-H-RAS P21 PROTEIN

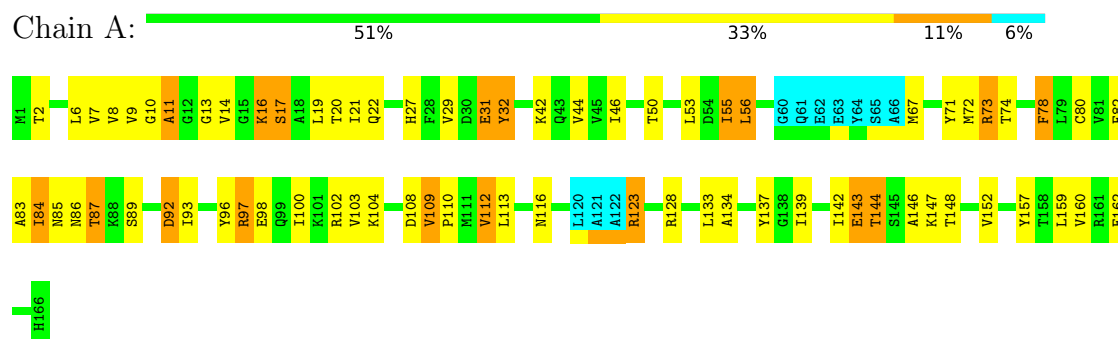


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

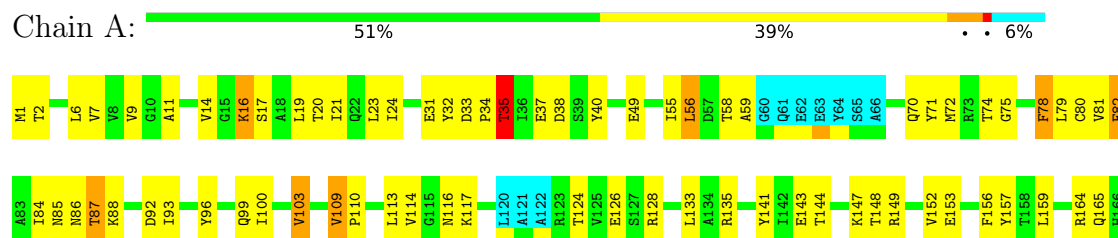
4.2.1 Score per residue for model 21

• Molecule 1: C-H-RAS P21 PROTEIN



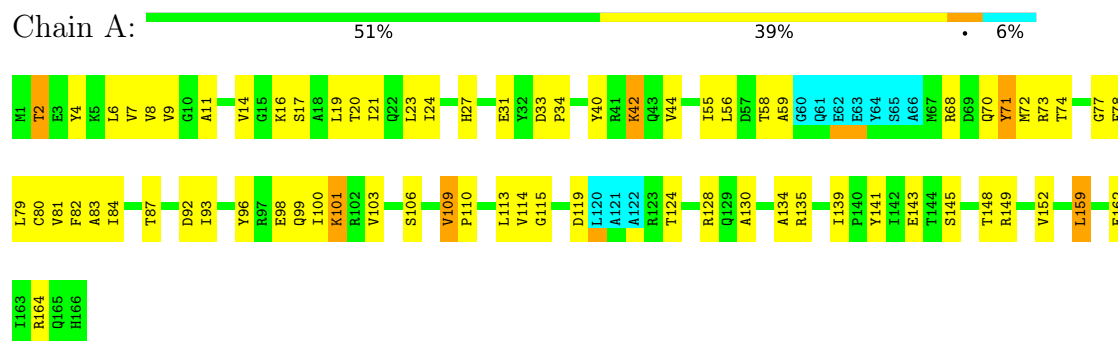
4.2.2 Score per residue for model 22

• Molecule 1: C-H-RAS P21 PROTEIN



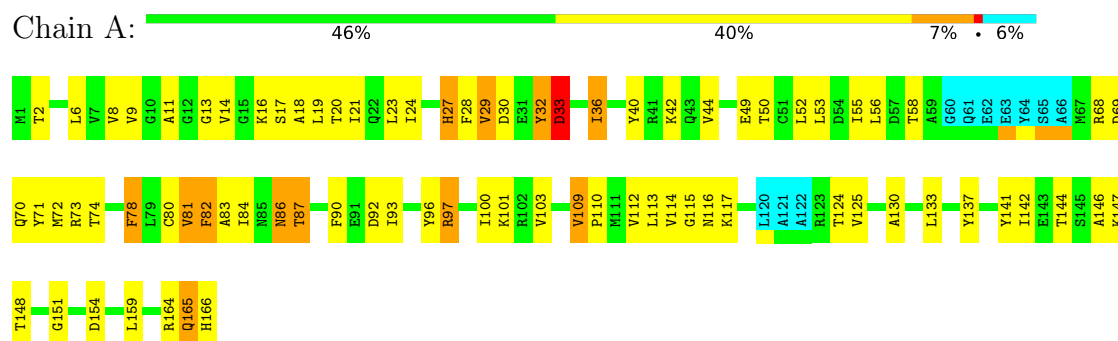
4.2.3 Score per residue for model 23

- Molecule 1: C-H-RAS P21 PROTEIN



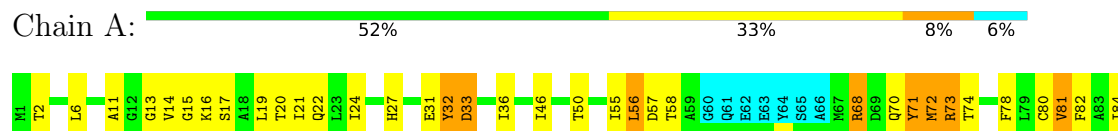
4.2.4 Score per residue for model 24

- Molecule 1: C-H-RAS P21 PROTEIN



4.2.5 Score per residue for model 25

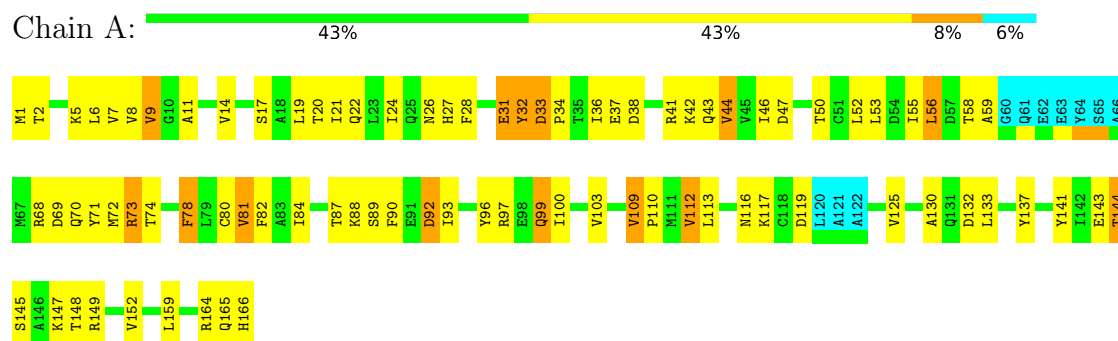
- Molecule 1: C-H-RAS P21 PROTEIN





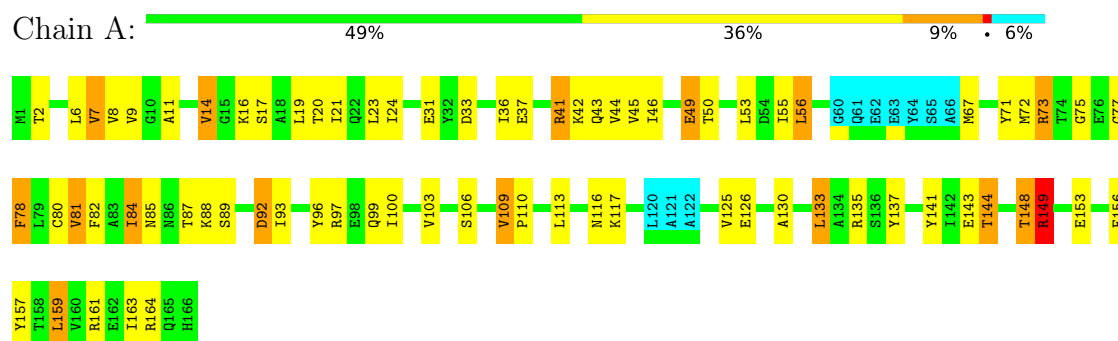
4.2.9 Score per residue for model 29

• Molecule 1: C-H-RAS P21 PROTEIN



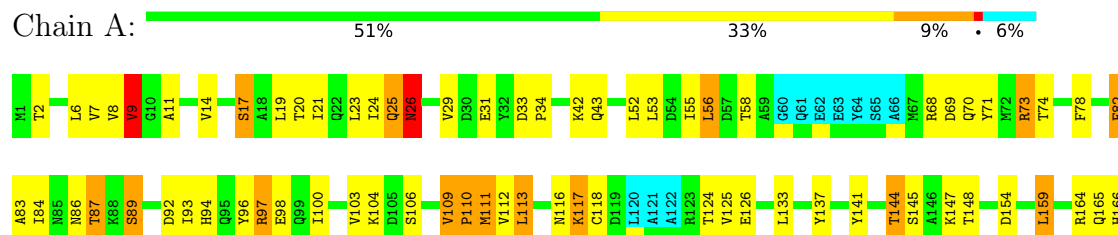
4.2.10 Score per residue for model 30

• Molecule 1: C-H-RAS P21 PROTEIN



4.2.11 Score per residue for model 31

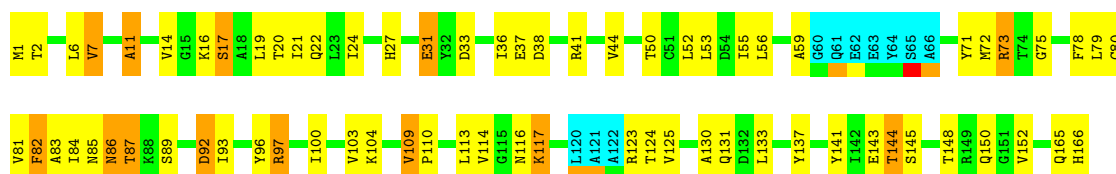
• Molecule 1: C-H-RAS P21 PROTEIN



4.2.12 Score per residue for model 32

• Molecule 1: C-H-RAS P21 PROTEIN

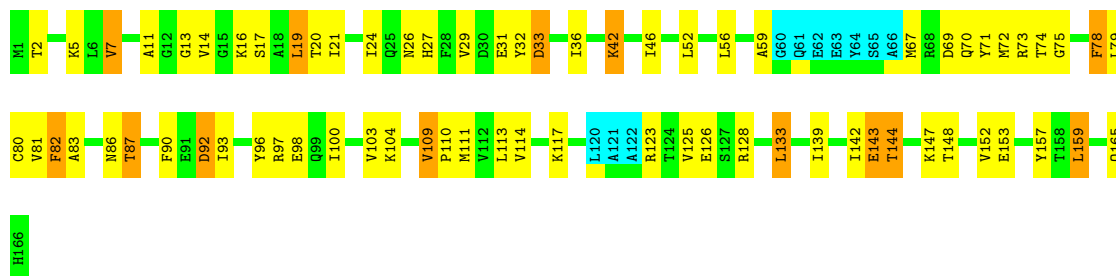




4.2.13 Score per residue for model 33

- Molecule 1: C-H-RAS P21 PROTEIN

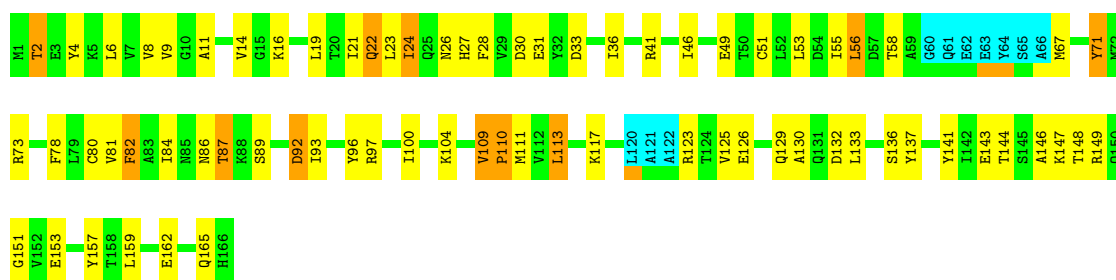
Chain A: 51% 35% 8% 6%



4.2.14 Score per residue for model 34

- Molecule 1: C-H-RAS P21 PROTEIN

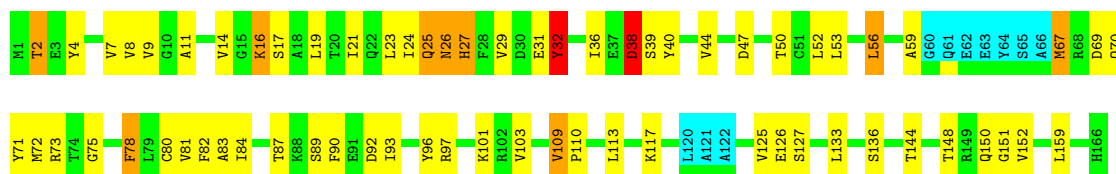
Chain A: 51% 37% 7% 6%



4.2.15 Score per residue for model 35

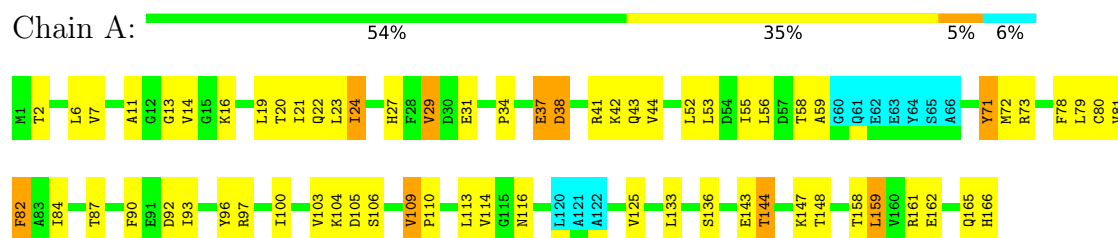
- Molecule 1: C-H-RAS P21 PROTEIN

Chain A: 54% 34% 5% 6%



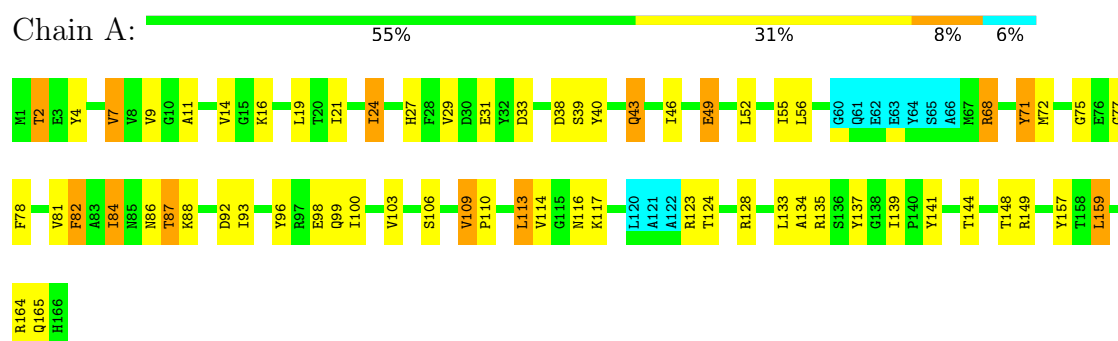
4.2.16 Score per residue for model 36

- Molecule 1: C-H-RAS P21 PROTEIN



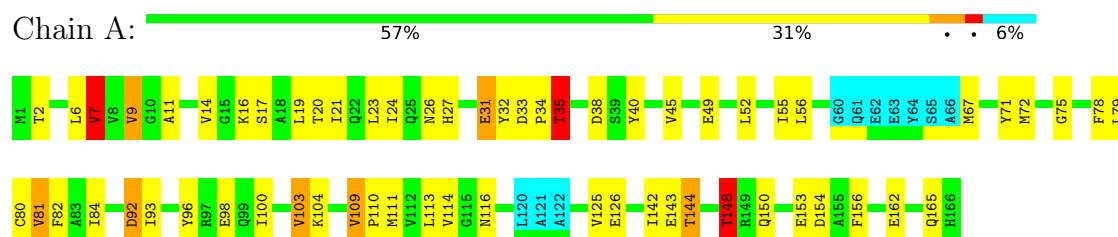
4.2.17 Score per residue for model 37 (medoid)

- Molecule 1: C-H-RAS P21 PROTEIN



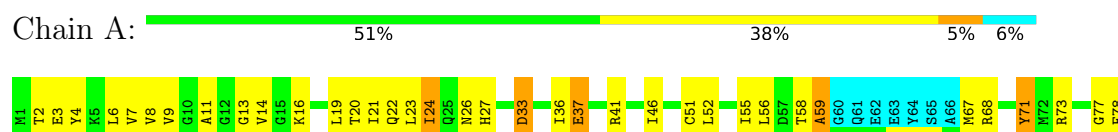
4.2.18 Score per residue for model 38

- Molecule 1: C-H-RAS P21 PROTEIN



4.2.19 Score per residue for model 39

- Molecule 1: C-H-RAS P21 PROTEIN

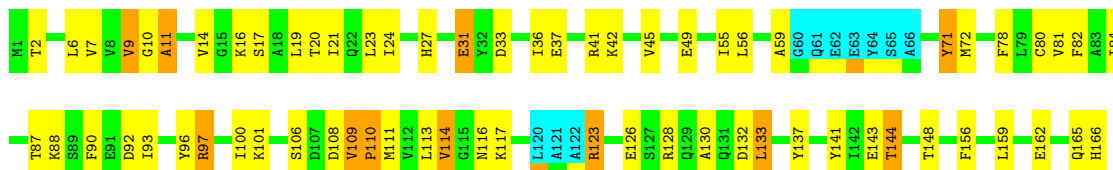




4.2.20 Score per residue for model 40

- Molecule 1: C-H-RAS P21 PROTEIN

Chain A: 54% 34% 7% 6%



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1.42±0.01	0±0/1269 (0.0± 0.0%)	1.15±0.01	1±1/1711 (0.0± 0.0%)
All	All	1.42	1/25380 (0.0%)	1.15	15/34220 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	114	VAL	C-N	-5.10	1.31	1.33	40	1

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	78	PHE	CA-CB-CG	-5.70	108.11	113.80	22	8
1	A	98	GLU	N-CA-C	-5.62	106.47	113.55	27	3
1	A	110	PRO	N-CA-C	-5.43	105.15	112.48	34	3
1	A	28	PHE	CA-CB-CG	-5.11	108.69	113.80	29	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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	1251	1233	1233	52±6
3	A	28	12	12	0±1
4	A	4	8	0	0±1
All	All	25680	25060	24900	1041

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:HG21	1:A:113:LEU:HD12	0.91	1.40	22	6
1:A:56:LEU:HD13	1:A:71:TYR:CE2	0.89	2.02	29	6
1:A:78:PHE:CE2	1:A:109:VAL:HG11	0.88	2.03	32	2
1:A:56:LEU:HD22	1:A:71:TYR:CG	0.88	2.04	29	10
1:A:93:ILE:HG21	1:A:113:LEU:HD13	0.88	1.42	30	15
1:A:56:LEU:HD22	1:A:71:TYR:CD2	0.86	2.04	35	7
1:A:109:VAL:HG12	1:A:110:PRO:HD2	0.86	1.46	27	20
1:A:6:LEU:HD12	1:A:55:ILE:HD12	0.86	1.45	26	3
1:A:56:LEU:HD13	1:A:71:TYR:CZ	0.86	2.06	34	11
1:A:6:LEU:HD12	1:A:55:ILE:CD1	0.83	2.03	26	3
1:A:93:ILE:HG21	1:A:113:LEU:CD1	0.83	2.03	40	12
1:A:90:PHE:CZ	1:A:133:LEU:HD13	0.83	2.08	36	2
1:A:11:ALA:HB3	1:A:14:VAL:CG1	0.79	2.07	30	20
1:A:20:THR:HG23	1:A:55:ILE:HG21	0.78	1.53	40	3
1:A:6:LEU:HD12	1:A:55:ILE:CG1	0.78	2.09	24	9
1:A:82:PHE:CE1	1:A:84:ILE:HG22	0.77	2.15	40	2
1:A:19:LEU:HD11	1:A:116:ASN:ND2	0.77	1.95	40	11
1:A:144:THR:HG22	1:A:151:GLY:C	0.77	2.05	25	7
1:A:56:LEU:HD22	1:A:71:TYR:CD1	0.77	2.15	37	9
1:A:20:THR:O	1:A:24:ILE:HD12	0.77	1.79	23	10
1:A:70:GLN:O	1:A:74:THR:HG23	0.76	1.80	23	7
1:A:6:LEU:HD12	1:A:55:ILE:HG12	0.75	1.58	34	7
1:A:17:SER:O	1:A:21:ILE:HD12	0.75	1.81	32	15
1:A:6:LEU:HD22	1:A:159:LEU:HD22	0.75	1.58	28	1
1:A:7:VAL:HG11	1:A:78:PHE:CE1	0.75	2.17	22	2
1:A:11:ALA:HB3	1:A:14:VAL:HG12	0.74	1.57	30	1
1:A:14:VAL:HA	1:A:83:ALA:HB2	0.74	1.60	23	5
1:A:7:VAL:HG11	1:A:78:PHE:CE2	0.74	2.17	35	1
1:A:79:LEU:HD11	1:A:155:ALA:HB1	0.74	1.60	27	3
1:A:81:VAL:O	1:A:93:ILE:HD11	0.73	1.83	40	6
1:A:19:LEU:HG	1:A:146:ALA:HB2	0.73	1.60	24	4
1:A:78:PHE:CE1	1:A:109:VAL:HG11	0.73	2.19	23	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HD23	1:A:141:TYR:CD1	0.73	2.18	25	5
1:A:6:LEU:CD2	1:A:159:LEU:HD22	0.73	2.13	39	4
1:A:20:THR:CG2	1:A:55:ILE:HG21	0.72	2.13	23	1
1:A:90:PHE:CZ	1:A:133:LEU:HD22	0.72	2.18	28	2
1:A:77:GLY:HA3	1:A:159:LEU:HD21	0.72	1.61	30	3
1:A:22:GLN:OE1	1:A:146:ALA:HB1	0.72	1.84	21	1
1:A:37:GLU:CG	1:A:59:ALA:HB3	0.72	2.15	40	2
1:A:34:PRO:O	1:A:35:THR:HG23	0.72	1.85	38	2
1:A:72:MET:HB2	1:A:103:VAL:HG21	0.71	1.62	30	6
1:A:56:LEU:HD22	1:A:71:TYR:CE2	0.71	2.20	31	3
1:A:130:ALA:HB1	1:A:141:TYR:CE1	0.71	2.20	30	6
1:A:36:ILE:O	1:A:59:ALA:HB3	0.71	1.86	35	1
1:A:19:LEU:HD22	1:A:152:VAL:HG22	0.70	1.60	32	3
1:A:16:LYS:HB3	1:A:81:VAL:HG21	0.70	1.61	28	10
1:A:19:LEU:CD2	1:A:152:VAL:HG22	0.69	2.17	29	10
1:A:78:PHE:CZ	1:A:100:ILE:HG23	0.69	2.21	36	13
1:A:6:LEU:HD12	1:A:55:ILE:HG13	0.69	1.65	31	6
1:A:109:VAL:HG12	1:A:110:PRO:CD	0.69	2.17	31	8
1:A:84:ILE:HD13	1:A:123:ARG:HG2	0.69	1.63	32	1
1:A:80:CYS:HB3	1:A:93:ILE:HD12	0.69	1.64	22	15
1:A:19:LEU:HD11	1:A:116:ASN:OD1	0.69	1.87	29	5
1:A:82:PHE:CZ	1:A:84:ILE:HG22	0.69	2.22	27	4
1:A:79:LEU:HD11	1:A:114:VAL:HG21	0.69	1.64	36	7
1:A:23:LEU:HD23	1:A:42:LYS:NZ	0.68	2.03	23	1
1:A:90:PHE:CE2	1:A:133:LEU:HD13	0.68	2.22	36	3
1:A:72:MET:C	1:A:103:VAL:HG11	0.68	2.14	29	3
1:A:56:LEU:HD13	1:A:71:TYR:CE1	0.68	2.24	37	4
1:A:78:PHE:CE2	1:A:100:ILE:HG23	0.68	2.24	30	6
1:A:29:VAL:HG21	1:A:32:TYR:HB3	0.68	1.65	24	1
1:A:72:MET:CB	1:A:103:VAL:HG21	0.67	2.18	22	12
1:A:142:ILE:HG21	1:A:154:ASP:OD1	0.67	1.90	24	2
1:A:99:GLN:O	1:A:103:VAL:HG23	0.67	1.88	23	7
1:A:44:VAL:O	1:A:50:THR:HG23	0.67	1.90	30	2
1:A:72:MET:HB3	1:A:103:VAL:HG21	0.66	1.68	22	8
1:A:93:ILE:HD13	1:A:96:TYR:CE2	0.66	2.25	31	1
1:A:16:LYS:CG	1:A:81:VAL:HG21	0.66	2.21	34	2
1:A:143:GLU:O	1:A:144:THR:HG23	0.66	1.91	40	9
1:A:11:ALA:HB3	1:A:14:VAL:HG13	0.65	1.66	35	13
1:A:34:PRO:O	1:A:59:ALA:HB1	0.65	1.91	23	4
1:A:41:ARG:HA	1:A:55:ILE:HD12	0.65	1.68	34	2
1:A:100:ILE:HD13	1:A:111:MET:HE1	0.65	1.68	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:H	1:A:21:ILE:HD12	0.64	1.51	34	3
1:A:6:LEU:HD13	1:A:156:PHE:CE1	0.64	2.28	38	3
1:A:16:LYS:CB	1:A:81:VAL:HG21	0.63	2.23	36	9
1:A:133:LEU:HD13	1:A:133:LEU:O	0.63	1.93	32	2
1:A:37:GLU:HB2	1:A:59:ALA:HB2	0.63	1.70	28	1
1:A:19:LEU:CD2	1:A:146:ALA:HB2	0.63	2.23	34	1
1:A:23:LEU:O	1:A:23:LEU:HD23	0.63	1.94	28	4
1:A:56:LEU:HD11	1:A:71:TYR:CG	0.63	2.29	25	1
1:A:8:VAL:O	1:A:9:VAL:HG13	0.62	1.95	31	8
1:A:2:THR:HG21	1:A:4:TYR:OH	0.62	1.93	35	3
1:A:97:ARG:NH1	1:A:139:ILE:HD13	0.62	2.08	27	1
1:A:45:VAL:HG13	1:A:49:GLU:O	0.62	1.95	40	2
1:A:97:ARG:NH1	1:A:139:ILE:HD11	0.62	2.09	33	1
1:A:16:LYS:HG2	1:A:81:VAL:HG21	0.62	1.72	34	5
1:A:21:ILE:HD13	1:A:29:VAL:HG21	0.61	1.71	33	4
1:A:7:VAL:HG22	1:A:75:GLY:HA3	0.61	1.72	30	6
1:A:6:LEU:HD22	1:A:159:LEU:HD13	0.61	1.72	25	4
1:A:100:ILE:HD13	1:A:111:MET:CE	0.61	2.24	31	1
1:A:19:LEU:HD21	1:A:152:VAL:HG22	0.61	1.72	33	2
1:A:158:THR:HG22	1:A:162:GLU:OE2	0.61	1.95	36	1
1:A:56:LEU:HD23	1:A:58:THR:HG22	0.61	1.71	34	1
1:A:84:ILE:HD12	1:A:84:ILE:O	0.61	1.95	34	1
1:A:78:PHE:CD2	1:A:100:ILE:HD13	0.60	2.31	24	7
1:A:14:VAL:HG12	1:A:89:SER:OG	0.60	1.95	34	4
1:A:43:GLN:OE1	1:A:52:LEU:HD12	0.60	1.96	37	1
1:A:16:LYS:HA	1:A:19:LEU:HD12	0.60	1.73	40	2
1:A:19:LEU:CG	1:A:146:ALA:HB2	0.60	2.26	34	2
1:A:21:ILE:HD12	1:A:21:ILE:N	0.59	2.12	39	3
1:A:18:ALA:HB2	1:A:29:VAL:HG12	0.59	1.74	28	2
1:A:134:ALA:HB1	1:A:139:ILE:HG13	0.59	1.73	21	3
1:A:18:ALA:CB	1:A:29:VAL:HG12	0.59	2.28	28	2
1:A:125:VAL:HG13	1:A:129:GLN:OE1	0.59	1.97	28	1
1:A:58:THR:HG22	1:A:68:ARG:HD3	0.59	1.75	28	1
1:A:22:GLN:NE2	1:A:152:VAL:HG21	0.59	2.13	29	1
1:A:84:ILE:O	1:A:125:VAL:HG23	0.59	1.97	29	7
1:A:24:ILE:N	1:A:24:ILE:HD13	0.59	2.13	28	1
1:A:79:LEU:CD1	1:A:114:VAL:HG21	0.58	2.28	36	4
1:A:33:ASP:CB	1:A:36:ILE:HD12	0.58	2.28	29	4
1:A:82:PHE:CB	1:A:113:LEU:HD11	0.58	2.28	35	2
1:A:37:GLU:HG2	1:A:59:ALA:HB3	0.58	1.76	22	2
1:A:84:ILE:HD12	1:A:123:ARG:HB2	0.58	1.75	40	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:GLN:OE1	1:A:50:THR:HG21	0.58	1.99	30	1
1:A:19:LEU:HD11	1:A:116:ASN:CG	0.58	2.24	31	2
1:A:78:PHE:CD1	1:A:100:ILE:HD13	0.57	2.34	37	2
1:A:33:ASP:O	1:A:36:ILE:HD11	0.57	1.98	24	1
1:A:42:LYS:HE3	1:A:44:VAL:HG13	0.57	1.75	29	1
1:A:29:VAL:HG13	1:A:30:ASP:N	0.57	2.14	24	2
1:A:37:GLU:HG3	1:A:59:ALA:HB3	0.57	1.75	40	1
1:A:42:LYS:HD3	1:A:44:VAL:HG13	0.57	1.75	23	3
1:A:44:VAL:CG2	1:A:53:LEU:HD12	0.57	2.29	29	2
1:A:58:THR:HG21	1:A:68:ARG:CD	0.57	2.30	39	1
1:A:17:SER:C	1:A:21:ILE:HD12	0.57	2.25	31	14
1:A:23:LEU:HD13	1:A:156:PHE:CE2	0.57	2.33	28	1
1:A:144:THR:HG22	1:A:151:GLY:O	0.57	2.00	35	4
1:A:36:ILE:O	1:A:59:ALA:HB2	0.56	2.01	33	1
1:A:77:GLY:CA	1:A:159:LEU:HD21	0.56	2.30	30	3
1:A:58:THR:HG21	1:A:68:ARG:CG	0.56	2.30	24	1
1:A:73:ARG:HG3	1:A:103:VAL:HG12	0.56	1.77	30	4
1:A:130:ALA:HB1	1:A:141:TYR:CE2	0.56	2.35	24	1
1:A:21:ILE:HD12	1:A:21:ILE:H	0.56	1.59	27	2
1:A:6:LEU:HD13	1:A:55:ILE:HG13	0.56	1.77	29	1
1:A:56:LEU:C	1:A:56:LEU:HD13	0.56	2.26	23	1
1:A:46:ILE:HD12	1:A:51:CYS:SG	0.56	2.41	39	2
1:A:21:ILE:HG21	1:A:27:HIS:NE2	0.56	2.16	28	2
1:A:133:LEU:C	1:A:133:LEU:HD13	0.56	2.26	21	3
1:A:90:PHE:CE1	1:A:133:LEU:HD22	0.55	2.36	35	1
1:A:23:LEU:HD23	1:A:42:LYS:HZ3	0.55	1.60	23	1
1:A:24:ILE:HG23	1:A:42:LYS:HD3	0.55	1.77	33	2
1:A:32:TYR:O	1:A:36:ILE:HD13	0.55	2.01	27	1
1:A:19:LEU:HD23	1:A:152:VAL:HG22	0.55	1.78	28	1
1:A:58:THR:HG21	1:A:68:ARG:HG3	0.55	1.76	23	3
1:A:15:GLY:O	1:A:19:LEU:HD12	0.55	2.02	26	3
1:A:93:ILE:HD13	1:A:96:TYR:CE1	0.55	2.36	27	1
1:A:159:LEU:C	1:A:159:LEU:HD13	0.55	2.26	29	2
1:A:20:THR:HG21	1:A:40:TYR:CD2	0.55	2.37	23	1
1:A:130:ALA:HB1	1:A:141:TYR:CZ	0.55	2.37	30	3
1:A:78:PHE:CD1	1:A:109:VAL:HG11	0.54	2.37	28	3
1:A:100:ILE:HG21	1:A:111:MET:HE1	0.54	1.77	31	1
1:A:40:TYR:O	1:A:55:ILE:HD12	0.54	2.02	22	3
1:A:83:ALA:HB1	1:A:117:LYS:HE2	0.54	1.79	35	1
1:A:19:LEU:HD11	1:A:116:ASN:HD22	0.54	1.62	39	3
1:A:21:ILE:HD11	1:A:32:TYR:CE1	0.54	2.38	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:HD11	1:A:32:TYR:CE2	0.54	2.37	35	1
1:A:56:LEU:HD13	1:A:71:TYR:CD2	0.54	2.38	26	2
1:A:159:LEU:CD2	1:A:163:ILE:HD11	0.53	2.33	30	1
1:A:4:TYR:HB2	1:A:53:LEU:HD23	0.53	1.80	34	1
1:A:7:VAL:HG12	1:A:68:ARG:HH22	0.53	1.63	37	1
1:A:80:CYS:CB	1:A:93:ILE:HD12	0.53	2.32	23	1
1:A:44:VAL:HG21	1:A:53:LEU:HD12	0.53	1.79	29	3
1:A:45:VAL:HG13	1:A:49:GLU:C	0.53	2.29	40	2
1:A:23:LEU:C	1:A:24:ILE:HD13	0.53	2.28	28	1
1:A:20:THR:HG22	1:A:24:ILE:HD11	0.53	1.81	31	1
1:A:97:ARG:NH2	1:A:133:LEU:HD12	0.53	2.18	33	1
1:A:6:LEU:HD11	1:A:53:LEU:HD22	0.53	1.79	31	2
1:A:38:ASP:OD1	1:A:67:MET:HE2	0.53	2.04	35	1
1:A:20:THR:HG22	1:A:24:ILE:CD1	0.53	2.32	31	5
1:A:56:LEU:HD11	1:A:71:TYR:CE2	0.53	2.39	38	2
1:A:82:PHE:CZ	1:A:125:VAL:HG11	0.53	2.38	36	2
1:A:125:VAL:HG13	1:A:129:GLN:NE2	0.53	2.19	34	1
1:A:97:ARG:HA	1:A:100:ILE:HD12	0.52	1.80	26	2
1:A:125:VAL:HG13	1:A:129:GLN:CD	0.52	2.29	28	2
1:A:53:LEU:HD21	1:A:160:VAL:HG21	0.52	1.80	21	1
1:A:6:LEU:HD13	1:A:156:PHE:CD1	0.52	2.39	26	2
1:A:78:PHE:HE2	1:A:109:VAL:HG11	0.52	1.64	26	1
1:A:7:VAL:HG12	1:A:68:ARG:NH2	0.52	2.19	37	1
1:A:159:LEU:C	1:A:159:LEU:HD23	0.52	2.29	35	3
1:A:112:VAL:CG2	1:A:159:LEU:HD22	0.52	2.34	31	1
1:A:130:ALA:HB3	1:A:141:TYR:CE2	0.52	2.39	40	1
1:A:11:ALA:HB2	1:A:92:ASP:OD2	0.52	2.04	28	1
1:A:133:LEU:HD13	1:A:133:LEU:C	0.52	2.30	32	1
1:A:114:VAL:CG1	1:A:144:THR:HG23	0.52	2.35	37	1
1:A:21:ILE:HG22	1:A:27:HIS:NE2	0.52	2.20	27	6
1:A:96:TYR:C	1:A:96:TYR:CD1	0.52	2.89	27	2
1:A:56:LEU:HD11	1:A:71:TYR:CZ	0.51	2.40	21	2
1:A:14:VAL:CG2	1:A:81:VAL:HG11	0.51	2.35	34	2
1:A:36:ILE:HD13	1:A:40:TYR:OH	0.51	2.06	35	1
1:A:33:ASP:HB2	1:A:36:ILE:HD12	0.51	1.83	40	5
1:A:97:ARG:HB2	1:A:111:MET:HE1	0.51	1.82	40	1
1:A:23:LEU:HD21	1:A:44:VAL:HG11	0.51	1.82	28	2
1:A:6:LEU:HD13	1:A:55:ILE:CD1	0.51	2.36	21	1
1:A:73:ARG:HD2	1:A:74:THR:HG23	0.51	1.83	21	1
1:A:73:ARG:N	1:A:103:VAL:HG11	0.51	2.21	29	7
1:A:33:ASP:HB3	1:A:36:ILE:HD11	0.51	1.81	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:THR:HG21	1:A:4:TYR:CZ	0.50	2.41	34	2
1:A:114:VAL:HG12	1:A:144:THR:OG1	0.50	2.06	38	1
1:A:11:ALA:O	1:A:14:VAL:HG22	0.50	2.07	26	1
1:A:93:ILE:CG2	1:A:113:LEU:HD13	0.50	2.28	30	4
1:A:82:PHE:HB2	1:A:113:LEU:HD11	0.50	1.83	35	1
1:A:56:LEU:HD22	1:A:71:TYR:CZ	0.50	2.42	31	1
1:A:32:TYR:CG	1:A:32:TYR:O	0.50	2.64	21	2
1:A:44:VAL:HG22	1:A:53:LEU:HD12	0.50	1.84	36	2
1:A:83:ALA:HB1	1:A:117:LYS:HD2	0.50	1.83	24	1
1:A:93:ILE:CG2	1:A:113:LEU:HD12	0.49	2.34	23	2
1:A:34:PRO:C	1:A:35:THR:HG23	0.49	2.32	26	1
1:A:46:ILE:O	1:A:46:ILE:HG22	0.49	2.06	28	1
1:A:23:LEU:HD23	1:A:42:LYS:HG2	0.49	1.83	40	1
1:A:83:ALA:HB3	1:A:86:ASN:ND2	0.49	2.22	32	2
3:A:200:GDP:PA	4:A:203:HOH:O	0.49	2.70	21	1
1:A:84:ILE:HD13	1:A:123:ARG:CG	0.49	2.37	32	1
1:A:46:ILE:HG23	1:A:157:TYR:CE2	0.49	2.42	21	1
1:A:14:VAL:HG21	1:A:81:VAL:HB	0.49	1.84	38	4
1:A:33:ASP:CB	1:A:36:ILE:HD11	0.49	2.38	27	1
1:A:8:VAL:HG12	1:A:16:LYS:NZ	0.48	2.23	21	1
1:A:36:ILE:HG21	1:A:40:TYR:OH	0.48	2.08	24	2
1:A:82:PHE:CE2	1:A:115:GLY:CA	0.48	2.96	25	1
1:A:112:VAL:CG2	1:A:159:LEU:HD23	0.48	2.38	29	1
1:A:27:HIS:CD2	1:A:27:HIS:C	0.48	2.91	28	4
1:A:59:ALA:HB2	4:A:205:HOH:O	0.48	2.09	40	1
1:A:73:ARG:CG	1:A:103:VAL:HG12	0.48	2.38	25	3
1:A:32:TYR:CE2	1:A:36:ILE:HD12	0.48	2.44	26	1
1:A:21:ILE:HD11	1:A:32:TYR:HD2	0.47	1.69	33	1
1:A:159:LEU:HD13	1:A:159:LEU:O	0.47	2.09	40	1
1:A:78:PHE:CZ	1:A:109:VAL:HG11	0.47	2.44	32	1
1:A:83:ALA:HB3	1:A:86:ASN:HD21	0.47	1.68	21	1
1:A:46:ILE:HG22	1:A:47:ASP:OD1	0.47	2.10	29	1
1:A:82:PHE:CE2	1:A:84:ILE:HG22	0.47	2.45	21	3
1:A:56:LEU:CD2	1:A:71:TYR:CD1	0.47	2.98	21	2
1:A:21:ILE:HA	1:A:24:ILE:HG12	0.47	1.87	36	5
1:A:100:ILE:HD12	1:A:111:MET:HE2	0.47	1.86	34	1
1:A:78:PHE:CZ	1:A:100:ILE:CG2	0.46	2.99	22	7
1:A:6:LEU:HD13	1:A:156:PHE:CE2	0.46	2.44	22	1
1:A:21:ILE:HD11	1:A:32:TYR:CD2	0.46	2.44	33	1
1:A:6:LEU:CD1	1:A:156:PHE:CE2	0.46	2.98	22	1
1:A:37:GLU:HB3	1:A:59:ALA:HB2	0.46	1.87	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ARG:NH1	1:A:137:TYR:CG	0.46	2.84	31	1
1:A:82:PHE:O	1:A:82:PHE:CG	0.46	2.68	39	15
1:A:78:PHE:CE2	1:A:100:ILE:CG2	0.46	2.98	32	5
1:A:11:ALA:HB2	1:A:89:SER:HA	0.46	1.87	31	4
1:A:32:TYR:CE2	1:A:36:ILE:CD1	0.46	2.99	26	2
1:A:130:ALA:CB	1:A:141:TYR:CZ	0.46	2.99	26	7
1:A:32:TYR:CD2	1:A:32:TYR:O	0.46	2.69	26	2
1:A:23:LEU:CD1	1:A:156:PHE:CD2	0.46	2.99	28	1
1:A:97:ARG:CZ	1:A:137:TYR:CD2	0.46	2.99	21	1
1:A:97:ARG:NH2	1:A:137:TYR:CD2	0.46	2.84	21	1
1:A:78:PHE:CD1	1:A:100:ILE:CD1	0.46	2.99	40	3
1:A:82:PHE:CE1	1:A:115:GLY:CA	0.46	2.99	23	2
1:A:56:LEU:HD11	1:A:71:TYR:CB	0.46	2.41	25	1
1:A:112:VAL:HG21	1:A:159:LEU:HD22	0.45	1.88	31	1
1:A:19:LEU:HD21	1:A:116:ASN:ND2	0.45	2.26	38	1
1:A:56:LEU:CD1	1:A:71:TYR:CE2	0.45	2.99	38	1
1:A:56:LEU:CB	1:A:71:TYR:CE2	0.45	2.99	22	1
1:A:56:LEU:CD1	1:A:71:TYR:CG	0.45	2.99	25	1
1:A:97:ARG:CZ	1:A:137:TYR:CD1	0.45	2.99	28	1
1:A:78:PHE:CD2	1:A:100:ILE:CD1	0.45	2.99	21	5
1:A:32:TYR:O	1:A:32:TYR:CG	0.45	2.69	27	4
1:A:97:ARG:CG	1:A:137:TYR:CE2	0.45	3.00	25	1
1:A:79:LEU:HD12	1:A:159:LEU:CD1	0.45	2.41	26	1
1:A:99:GLN:OE1	1:A:103:VAL:HG23	0.45	2.12	29	1
1:A:14:VAL:HG22	1:A:16:LYS:HG3	0.45	1.89	30	1
1:A:118:CYS:HG	1:A:144:THR:C	0.45	2.20	31	1
1:A:37:GLU:HB2	1:A:59:ALA:HB3	0.45	1.89	32	1
1:A:82:PHE:HZ	1:A:125:VAL:HG11	0.45	1.72	32	2
1:A:21:ILE:HG21	1:A:29:VAL:HG11	0.45	1.87	36	1
1:A:9:VAL:HG23	1:A:80:CYS:HA	0.45	1.88	22	1
1:A:41:ARG:CA	1:A:55:ILE:HD12	0.45	2.41	34	1
1:A:97:ARG:NH2	1:A:137:TYR:CE1	0.45	2.85	34	1
1:A:113:LEU:HD23	1:A:141:TYR:HD1	0.45	1.64	37	1
1:A:56:LEU:CD2	1:A:71:TYR:CG	0.44	3.00	27	2
1:A:44:VAL:HG22	1:A:53:LEU:HD13	0.44	1.87	32	1
1:A:78:PHE:CD1	1:A:109:VAL:CG1	0.44	3.00	35	1
1:A:78:PHE:CG	1:A:100:ILE:HD13	0.44	2.47	40	1
1:A:56:LEU:HD23	1:A:57:ASP:N	0.44	2.27	25	1
1:A:27:HIS:CD2	1:A:27:HIS:O	0.44	2.70	38	6
1:A:44:VAL:HG22	1:A:53:LEU:CD1	0.44	2.42	32	2
1:A:73:ARG:HG2	1:A:103:VAL:HG12	0.44	1.88	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:HD22	1:A:71:TYR:CB	0.44	2.41	29	3
1:A:17:SER:CB	1:A:32:TYR:CE1	0.44	3.01	27	1
1:A:148:THR:O	1:A:149:ARG:CB	0.44	2.65	30	1
1:A:36:ILE:C	1:A:59:ALA:HB3	0.44	2.37	35	1
3:A:200:GDP:PB	4:A:203:HOH:O	0.44	2.74	21	1
1:A:97:ARG:CZ	1:A:137:TYR:CE2	0.44	2.99	24	1
1:A:56:LEU:CD1	1:A:71:TYR:CE1	0.44	3.00	21	2
1:A:6:LEU:HD22	1:A:159:LEU:CD1	0.44	2.40	25	1
1:A:36:ILE:HG22	1:A:37:GLU:N	0.44	2.28	39	1
3:A:200:GDP:PB	4:A:205:HOH:O	0.44	2.75	21	1
1:A:79:LEU:CD1	1:A:159:LEU:HD13	0.44	2.42	26	1
1:A:73:ARG:HB3	1:A:103:VAL:HG13	0.44	1.89	29	1
1:A:78:PHE:CD2	1:A:109:VAL:HG11	0.44	2.47	29	1
1:A:137:TYR:N	1:A:137:TYR:CD1	0.44	2.85	37	1
1:A:84:ILE:HD12	1:A:123:ARG:CB	0.44	2.43	40	1
1:A:97:ARG:NH2	1:A:137:TYR:CZ	0.43	2.86	30	1
1:A:6:LEU:HD23	1:A:159:LEU:HD13	0.43	1.90	21	1
1:A:130:ALA:HB3	1:A:141:TYR:CZ	0.43	2.48	34	1
1:A:32:TYR:C	1:A:32:TYR:CD1	0.43	2.95	35	2
1:A:86:ASN:OD1	1:A:87:THR:N	0.43	2.51	25	1
1:A:81:VAL:HG12	1:A:82:PHE:N	0.43	2.28	40	2
1:A:78:PHE:CZ	1:A:100:ILE:HG21	0.43	2.49	27	1
1:A:92:ASP:O	1:A:96:TYR:CD1	0.43	2.72	34	10
1:A:7:VAL:HG21	1:A:78:PHE:HE1	0.43	1.74	32	1
1:A:90:PHE:CE2	1:A:133:LEU:CD1	0.43	3.00	24	1
1:A:83:ALA:HB1	1:A:117:LYS:HE3	0.43	1.89	33	1
1:A:130:ALA:CB	1:A:141:TYR:CE2	0.43	3.01	40	1
1:A:97:ARG:NH2	1:A:137:TYR:CE2	0.43	2.86	24	1
1:A:21:ILE:HA	1:A:24:ILE:CG1	0.43	2.44	27	1
1:A:32:TYR:O	1:A:32:TYR:CD1	0.43	2.71	24	2
1:A:98:GLU:O	1:A:101:LYS:CG	0.43	2.67	23	1
1:A:16:LYS:HG3	1:A:81:VAL:HG21	0.43	1.91	34	1
1:A:6:LEU:HD23	1:A:159:LEU:HD22	0.43	1.85	39	1
1:A:20:THR:O	1:A:24:ILE:HG12	0.43	2.14	27	3
1:A:97:ARG:NH2	1:A:133:LEU:CD1	0.43	2.82	33	1
1:A:111:MET:HB3	1:A:139:ILE:HG21	0.42	1.91	33	1
1:A:44:VAL:HG21	1:A:53:LEU:CD1	0.42	2.44	35	1
1:A:27:HIS:CD2	1:A:27:HIS:N	0.42	2.86	25	3
1:A:92:ASP:O	1:A:96:TYR:CD2	0.42	2.73	21	8
1:A:21:ILE:HD13	1:A:29:VAL:CG2	0.42	2.43	33	1
1:A:14:VAL:HG21	1:A:81:VAL:CG1	0.42	2.44	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LEU:HD23	1:A:71:TYR:CZ	0.42	2.49	23	1
1:A:93:ILE:HD13	1:A:96:TYR:CZ	0.42	2.49	31	1
1:A:20:THR:C	1:A:24:ILE:HD12	0.42	2.39	33	1
1:A:42:LYS:HE2	1:A:44:VAL:HG11	0.42	1.91	21	1
1:A:86:ASN:O	1:A:87:THR:CB	0.42	2.68	34	11
1:A:45:VAL:HG12	1:A:46:ILE:N	0.42	2.30	30	1
1:A:7:VAL:HG21	1:A:78:PHE:CE1	0.42	2.49	32	1
1:A:90:PHE:CZ	1:A:133:LEU:CB	0.42	3.03	40	1
1:A:14:VAL:HG23	1:A:81:VAL:HG11	0.42	1.90	34	1
1:A:1:MET:HE1	1:A:43:GLN:OE1	0.42	2.15	29	1
1:A:93:ILE:CG2	1:A:97:ARG:CZ	0.42	2.97	33	1
1:A:9:VAL:HG21	1:A:72:MET:HE2	0.42	1.91	40	1
1:A:50:THR:HG22	1:A:51:CYS:N	0.42	2.29	28	1
1:A:59:ALA:HB1	4:A:204:HOH:O	0.42	2.14	39	1
1:A:21:ILE:CG2	1:A:27:HIS:NE2	0.42	2.82	37	12
1:A:97:ARG:CD	1:A:137:TYR:CE2	0.42	3.02	32	1
1:A:56:LEU:HD21	1:A:71:TYR:CG	0.42	2.50	33	1
1:A:114:VAL:CG1	1:A:144:THR:HG22	0.42	2.45	33	1
1:A:73:ARG:HG3	1:A:74:THR:HG23	0.41	1.91	33	1
1:A:37:GLU:HB3	1:A:59:ALA:HB3	0.41	1.90	36	1
1:A:82:PHE:CD2	1:A:82:PHE:O	0.41	2.73	23	1
1:A:114:VAL:HG12	1:A:115:GLY:N	0.41	2.30	24	1
1:A:33:ASP:CB	1:A:36:ILE:CD1	0.41	2.98	30	3
1:A:17:SER:CB	4:A:203:HOH:O	0.41	2.68	21	1
1:A:92:ASP:O	1:A:96:TYR:CG	0.41	2.73	29	3
1:A:133:LEU:O	1:A:137:TYR:CD1	0.41	2.73	29	2
1:A:50:THR:HG22	1:A:50:THR:O	0.41	2.15	21	1
1:A:5:LYS:C	1:A:6:LEU:HD12	0.41	2.39	29	1
1:A:31:GLU:O	1:A:32:TYR:C	0.41	2.63	29	1
1:A:17:SER:N	4:A:202:HOH:O	0.41	2.54	31	1
1:A:4:TYR:CD1	1:A:4:TYR:N	0.41	2.87	39	2
1:A:90:PHE:CZ	1:A:133:LEU:CD2	0.41	3.00	28	1
1:A:148:THR:HG23	1:A:150:GLN:HB2	0.41	1.92	38	1
1:A:82:PHE:CD1	1:A:82:PHE:C	0.41	2.98	33	5
1:A:165:GLN:CG	1:A:166:HIS:N	0.41	2.84	28	3
1:A:79:LEU:HD12	1:A:159:LEU:HD11	0.41	1.92	26	2
1:A:133:LEU:O	1:A:137:TYR:CE2	0.41	2.74	30	1
1:A:14:VAL:CG2	1:A:81:VAL:CG1	0.41	2.98	33	2
1:A:114:VAL:HG13	1:A:144:THR:HG23	0.41	1.93	37	1
1:A:153:GLU:O	1:A:157:TYR:CD1	0.41	2.74	22	4
1:A:37:GLU:CG	1:A:59:ALA:CB	0.41	2.99	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLN:O	1:A:26:ASN:CB	0.41	2.68	31	2
1:A:22:GLN:NE2	1:A:149:ARG:CG	0.41	2.84	34	1
1:A:16:LYS:N	3:A:200:GDP:O2B	0.41	2.54	21	1
1:A:28:PHE:CD1	1:A:146:ALA:O	0.41	2.74	34	2
1:A:21:ILE:CA	1:A:24:ILE:HG12	0.41	2.46	27	1
1:A:94:HIS:O	1:A:94:HIS:CG	0.41	2.74	31	1
1:A:22:GLN:OE1	1:A:152:VAL:HG21	0.41	2.15	32	1
1:A:70:GLN:HA	1:A:73:ARG:HG2	0.41	1.92	33	1
1:A:90:PHE:CZ	1:A:133:LEU:HD23	0.41	2.51	33	1
1:A:142:ILE:HG22	1:A:143:GLU:H	0.41	1.76	33	1
1:A:82:PHE:CD2	1:A:114:VAL:O	0.41	2.74	40	1
1:A:108:ASP:OD1	1:A:166:HIS:CE1	0.41	2.74	40	1
1:A:23:LEU:HD13	1:A:156:PHE:CD2	0.41	2.50	28	1
1:A:33:ASP:N	1:A:34:PRO:CD	0.41	2.84	31	1
1:A:32:TYR:O	1:A:32:TYR:CD2	0.41	2.74	38	1
1:A:13:GLY:CA	3:A:200:GDP:O3B	0.40	2.69	21	1
1:A:56:LEU:CD2	1:A:71:TYR:CE2	0.40	3.00	31	1
1:A:133:LEU:O	1:A:137:TYR:CG	0.40	2.74	40	1
1:A:93:ILE:CG2	1:A:97:ARG:NH2	0.40	2.84	25	1
1:A:28:PHE:CE2	1:A:30:ASP:OD1	0.40	2.75	34	1
1:A:46:ILE:O	1:A:157:TYR:CE2	0.40	2.74	37	1
1:A:8:VAL:HG12	1:A:16:LYS:HZ1	0.40	1.76	21	1
1:A:32:TYR:CD1	1:A:32:TYR:C	0.40	3.00	21	1
1:A:24:ILE:HG12	1:A:42:LYS:CB	0.40	2.46	23	1
1:A:98:GLU:CG	1:A:99:GLN:N	0.40	2.85	25	1
1:A:17:SER:HB2	1:A:32:TYR:CE1	0.40	2.52	27	1
1:A:56:LEU:CD2	1:A:71:TYR:CD2	0.40	3.00	31	1
1:A:97:ARG:CZ	1:A:97:ARG:CB	0.40	2.98	24	1
1:A:39:SER:O	1:A:40:TYR:CG	0.40	2.75	35	1
1:A:39:SER:C	1:A:40:TYR:CD1	0.40	3.00	37	1
1:A:77:GLY:HA2	1:A:159:LEU:HD21	0.40	1.92	37	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	154/166 (93%)	119±3 (77±2%)	29±3 (19±2%)	6±2 (4±2%)	4	32
All	All	3080/3320 (93%)	2379 (77%)	587 (19%)	114 (4%)	4	32

All 37 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	31	GLU	15
1	A	7	VAL	9
1	A	148	THR	7
1	A	26	ASN	7
1	A	33	ASP	6
1	A	38	ASP	6
1	A	13	GLY	5
1	A	50	THR	5
1	A	112	VAL	4
1	A	58	THR	4
1	A	49	GLU	4
1	A	9	VAL	4
1	A	11	ALA	3
1	A	86	ASN	3
1	A	126	GLU	3
1	A	10	GLY	2
1	A	35	THR	2
1	A	46	ILE	2
1	A	59	ALA	2
1	A	32	TYR	2
1	A	25	GLN	2
1	A	67	MET	2
1	A	84	ILE	1
1	A	108	ASP	1
1	A	123	ARG	1
1	A	128	ARG	1
1	A	29	VAL	1
1	A	30	ASP	1
1	A	119	ASP	1
1	A	149	ARG	1
1	A	80	CYS	1
1	A	24	ILE	1
1	A	75	GLY	1
1	A	127	SER	1
1	A	103	VAL	1
1	A	153	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	165	GLN	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	138/144 (96%)	114±4 (82±3%)	24±4 (18±3%)	4	37
All	All	2760/2880 (96%)	2275 (82%)	485 (18%)	4	37

All 91 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	2	THR	20
1	A	109	VAL	20
1	A	87	THR	19
1	A	148	THR	15
1	A	165	GLN	14
1	A	147	LYS	12
1	A	159	LEU	12
1	A	97	ARG	11
1	A	104	LYS	11
1	A	82	PHE	11
1	A	164	ARG	11
1	A	52	LEU	11
1	A	73	ARG	10
1	A	144	THR	10
1	A	71	TYR	9
1	A	56	LEU	8
1	A	117	LYS	8
1	A	133	LEU	8
1	A	149	ARG	8
1	A	9	VAL	7
1	A	92	ASP	7
1	A	128	ARG	7
1	A	33	ASP	7
1	A	88	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	124	THR	7
1	A	126	GLU	7
1	A	106	SER	7
1	A	41	ARG	7
1	A	31	GLU	6
1	A	123	ARG	6
1	A	162	GLU	6
1	A	23	LEU	6
1	A	24	ILE	6
1	A	67	MET	5
1	A	38	ASP	5
1	A	84	ILE	5
1	A	135	ARG	5
1	A	101	LYS	5
1	A	69	ASP	5
1	A	81	VAL	5
1	A	22	GLN	5
1	A	132	ASP	5
1	A	136	SER	5
1	A	7	VAL	5
1	A	32	TYR	4
1	A	98	GLU	4
1	A	143	GLU	4
1	A	49	GLU	4
1	A	145	SER	4
1	A	29	VAL	4
1	A	111	MET	4
1	A	113	LEU	4
1	A	150	GLN	4
1	A	166	HIS	4
1	A	16	LYS	3
1	A	17	SER	3
1	A	89	SER	3
1	A	103	VAL	3
1	A	42	LYS	3
1	A	68	ARG	3
1	A	99	GLN	3
1	A	161	ARG	3
1	A	37	GLU	3
1	A	43	GLN	3
1	A	55	ILE	2
1	A	102	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	142	ILE	2
1	A	1	MET	2
1	A	35	THR	2
1	A	27	HIS	2
1	A	72	MET	2
1	A	105	ASP	2
1	A	70	GLN	2
1	A	129	GLN	2
1	A	19	LEU	2
1	A	26	ASN	2
1	A	112	VAL	1
1	A	36	ILE	1
1	A	153	GLU	1
1	A	94	HIS	1
1	A	25	GLN	1
1	A	96	TYR	1
1	A	44	VAL	1
1	A	14	VAL	1
1	A	85	ASN	1
1	A	154	ASP	1
1	A	131	GLN	1
1	A	5	LYS	1
1	A	47	ASP	1
1	A	3	GLU	1
1	A	91	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided