



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:51 pm GMT

PDB ID : 1Z6C
Title : Solution structure of an EGF pair (EGF34) from vitamin K-dependent protein S
Authors : Drakenberg, T.; Ghasriani, H.; Thulin, E.; Thamlitz, A.M.; Muranyi, A.; Annila, A.; Stenflo, J.
Deposited on : 2005-03-22

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

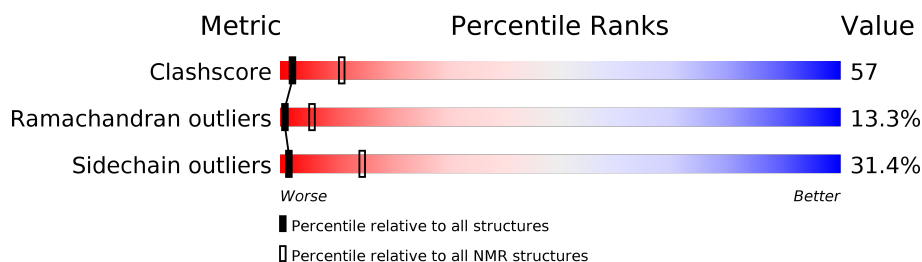
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	87	<div> <div>15%</div> <div>61%</div> <div>21%</div> <div>.</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:160-A:243 (84)	0.61	18

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

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

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

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1279 atoms, of which 615 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vitamin K-dependent protein S.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1271	402	611	106	139	13	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is water.

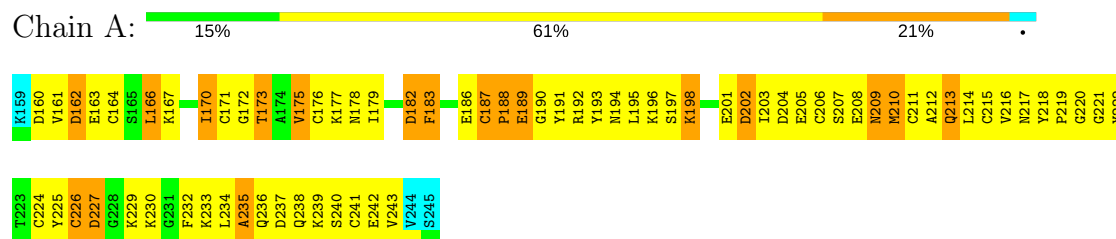
Mol	Chain	Residues	Atoms		
3	A	2	Total	H	O
			6	4	2

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: Vitamin K-dependent protein S

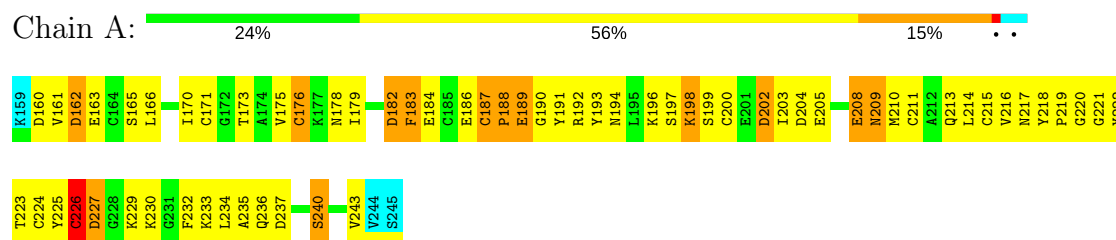


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

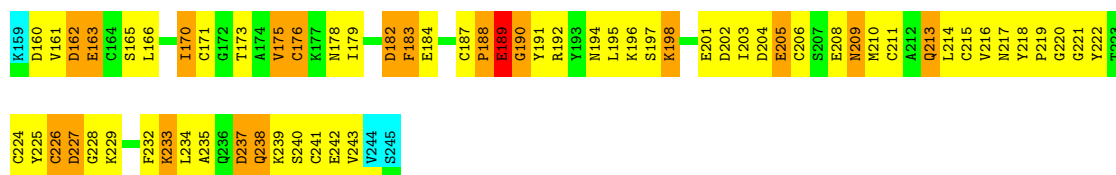
- Molecule 1: Vitamin K-dependent protein S



4.2.2 Score per residue for model 2

- Molecule 1: Vitamin K-dependent protein S

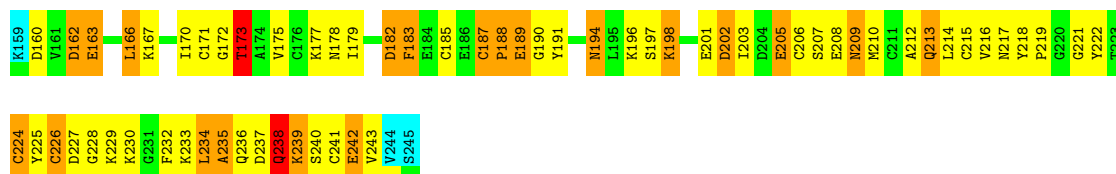




4.2.3 Score per residue for model 3

- Molecule 1: Vitamin K-dependent protein S

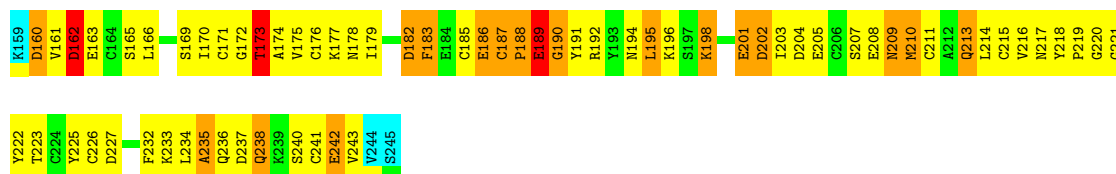
Chain A: 24% 47% 23%



4.2.4 Score per residue for model 4

- Molecule 1: Vitamin K-dependent protein S

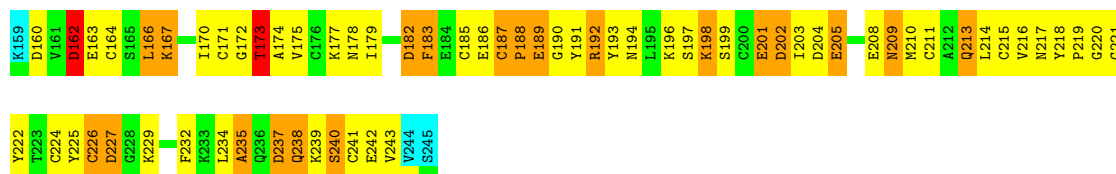
Chain A: 21% 53% 20%



4.2.5 Score per residue for model 5

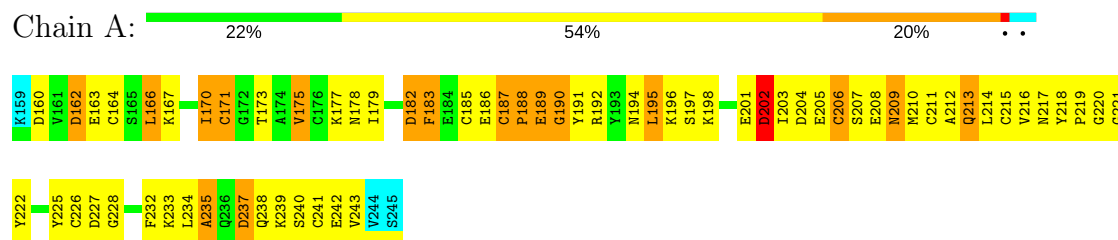
- Molecule 1: Vitamin K-dependent protein S

Chain A: 22% 49% 23%



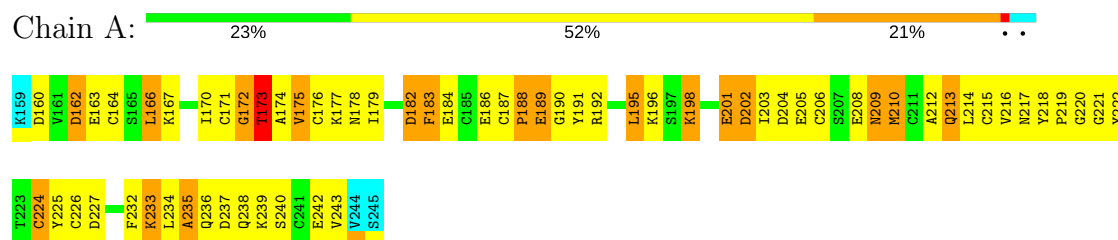
4.2.6 Score per residue for model 6

- Molecule 1: Vitamin K-dependent protein S



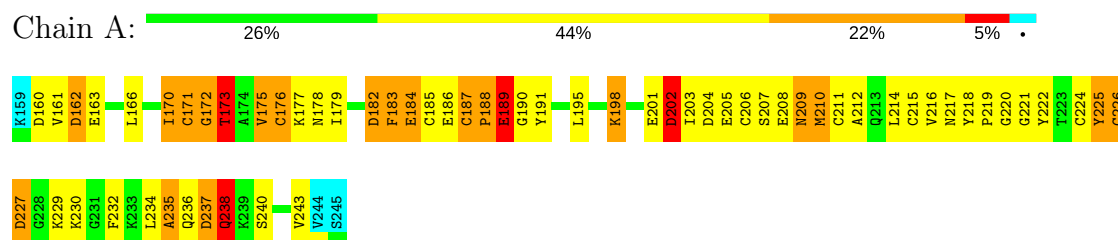
4.2.7 Score per residue for model 7

- Molecule 1: Vitamin K-dependent protein S



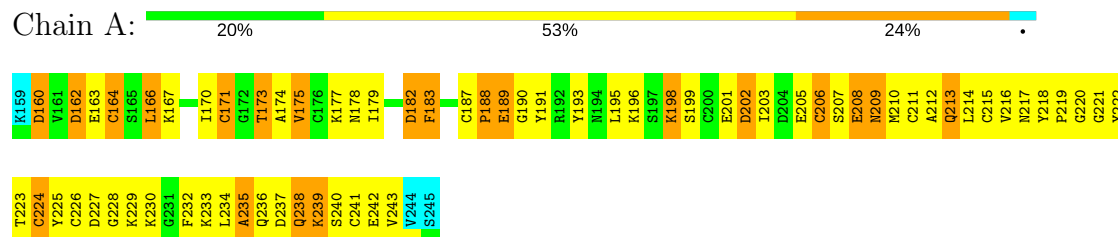
4.2.8 Score per residue for model 8

- Molecule 1: Vitamin K-dependent protein S



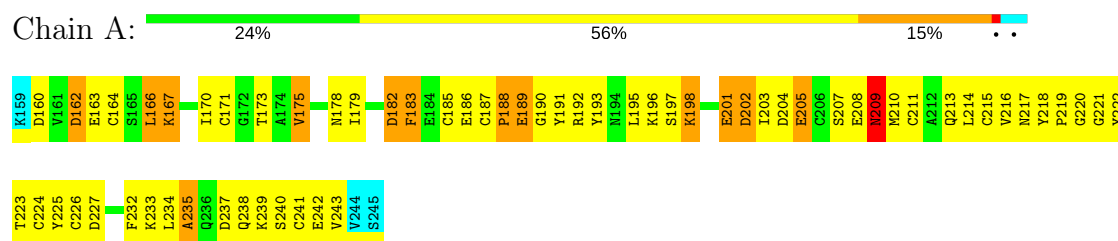
4.2.9 Score per residue for model 9

- Molecule 1: Vitamin K-dependent protein S



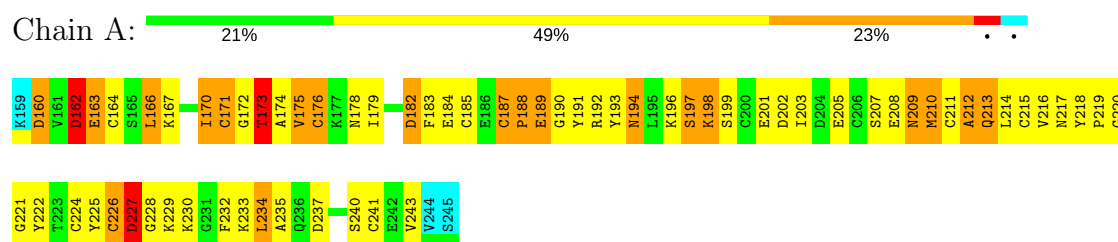
4.2.10 Score per residue for model 10

- Molecule 1: Vitamin K-dependent protein S



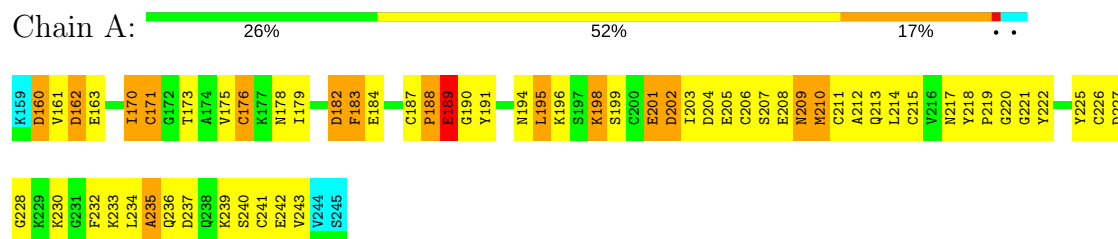
4.2.11 Score per residue for model 11

- Molecule 1: Vitamin K-dependent protein S



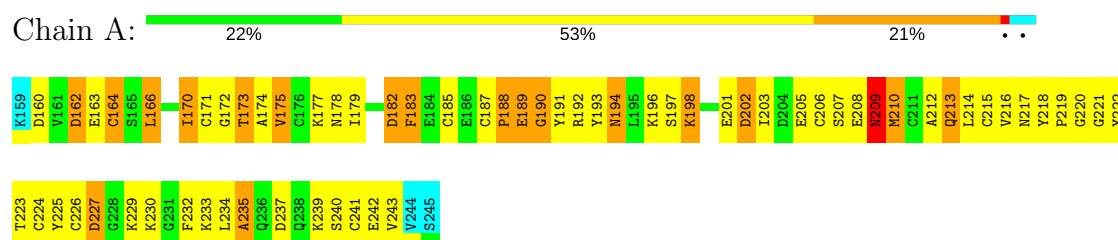
4.2.12 Score per residue for model 12

- Molecule 1: Vitamin K-dependent protein S



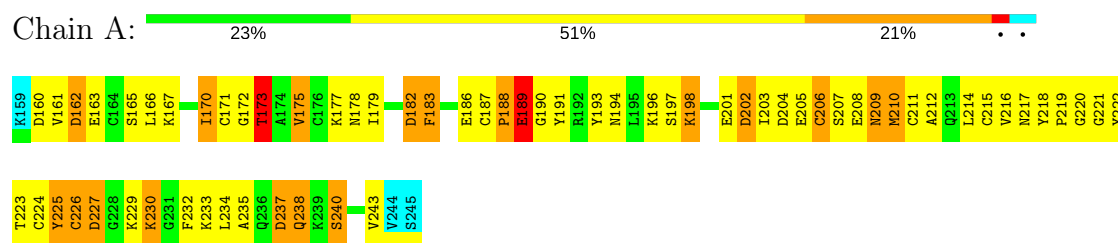
4.2.13 Score per residue for model 13

- Molecule 1: Vitamin K-dependent protein S



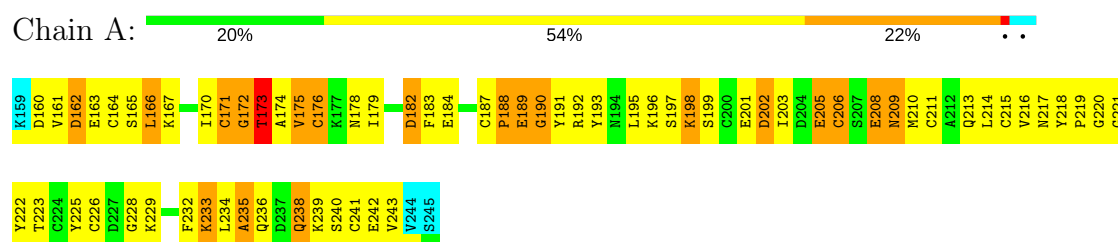
4.2.14 Score per residue for model 14

- Molecule 1: Vitamin K-dependent protein S



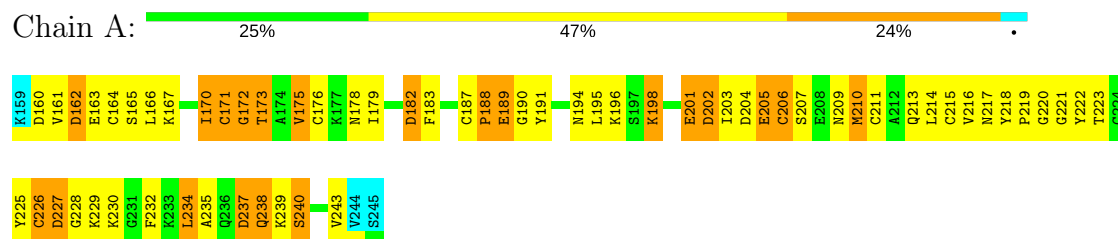
4.2.15 Score per residue for model 15

- Molecule 1: Vitamin K-dependent protein S



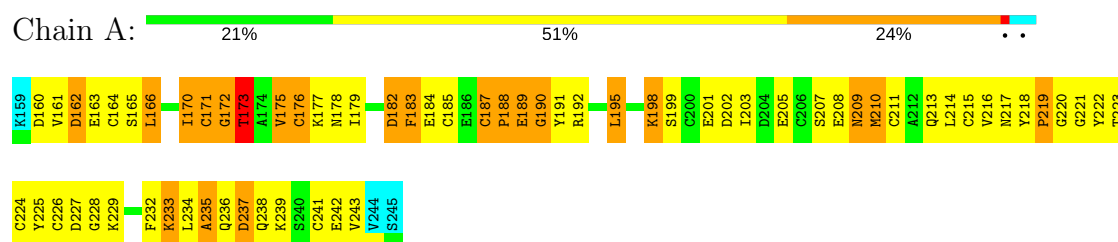
4.2.16 Score per residue for model 16

- Molecule 1: Vitamin K-dependent protein S



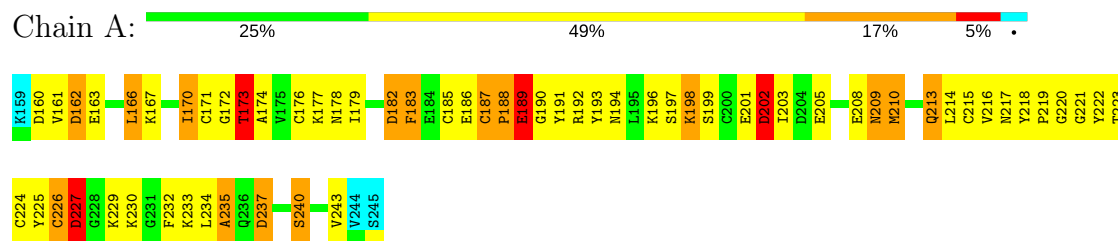
4.2.17 Score per residue for model 17

- Molecule 1: Vitamin K-dependent protein S



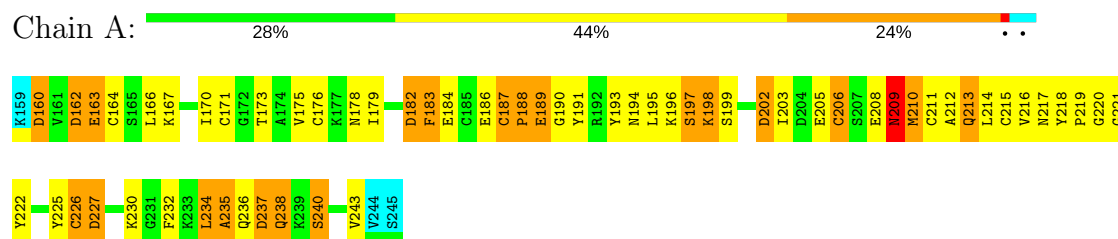
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Vitamin K-dependent protein S



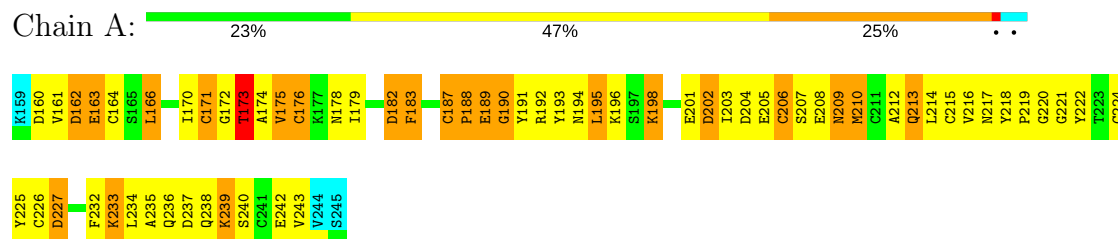
4.2.19 Score per residue for model 19

- Molecule 1: Vitamin K-dependent protein S



4.2.20 Score per residue for model 20

- Molecule 1: Vitamin K-dependent protein S



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Simulated annealing Torsion angle dynamics*.

Of the 200 calculated structures, 20 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. 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:
CA

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	637	582	582	69±5
3	A	2	4	0	1±1
All	All	12820	11720	11640	1386

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:218:TYR:O	3:A:249:HOH:O	1.10	1.64	2	12
1:A:214:LEU:HB2	1:A:225:TYR:HB2	0.97	1.35	12	1
1:A:161:VAL:O	3:A:248:HOH:O	0.96	1.82	16	1
1:A:170:ILE:HG23	1:A:183:PHE:CD2	0.94	1.96	20	7
1:A:189:GLU:O	1:A:191:TYR:N	0.92	2.02	13	7
1:A:214:LEU:HD23	1:A:225:TYR:HB3	0.91	1.41	12	1
1:A:190:GLY:O	1:A:203:ILE:HD12	0.88	1.66	7	15
1:A:216:VAL:HG23	1:A:225:TYR:CE1	0.87	2.04	1	19
1:A:232:PHE:HB2	1:A:243:VAL:HA	0.83	1.50	1	20
1:A:162:ASP:O	1:A:166:LEU:HD12	0.83	1.73	9	9
1:A:214:LEU:HD23	1:A:226:CYS:O	0.83	1.72	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:ALA:HB2	1:A:193:TYR:CD2	0.79	2.12	20	2
1:A:162:ASP:CB	1:A:166:LEU:HD12	0.79	2.08	18	6
1:A:226:CYS:HB3	1:A:232:PHE:CE2	0.78	2.13	11	7
1:A:214:LEU:HD12	1:A:225:TYR:CZ	0.76	2.15	8	2
1:A:214:LEU:HD23	1:A:225:TYR:CB	0.76	2.10	12	1
1:A:197:SER:O	1:A:198:LYS:HD2	0.76	1.81	19	2
1:A:213:GLN:C	1:A:214:LEU:HD22	0.76	2.01	13	16
1:A:214:LEU:HB2	1:A:225:TYR:O	0.75	1.79	11	6
1:A:226:CYS:HB3	1:A:232:PHE:CE1	0.74	2.17	8	5
1:A:227:ASP:HA	1:A:232:PHE:H	0.73	1.43	18	9
1:A:164:CYS:HA	1:A:170:ILE:HG21	0.73	1.61	16	3
1:A:214:LEU:HB3	1:A:225:TYR:CZ	0.73	2.19	20	18
1:A:187:CYS:O	1:A:189:GLU:N	0.72	2.22	13	14
1:A:179:ILE:HD11	1:A:182:ASP:CB	0.72	2.15	7	20
1:A:162:ASP:HB2	1:A:166:LEU:HD12	0.70	1.62	18	4
1:A:167:LYS:HB2	1:A:170:ILE:HD11	0.69	1.64	10	3
1:A:203:ILE:HG23	1:A:205:GLU:HG3	0.69	1.63	5	9
1:A:190:GLY:O	1:A:203:ILE:HB	0.68	1.88	12	19
1:A:226:CYS:CB	1:A:232:PHE:CE2	0.68	2.75	11	4
1:A:214:LEU:HD12	1:A:225:TYR:OH	0.68	1.88	8	2
1:A:212:ALA:HB3	1:A:241:CYS:SG	0.68	2.29	12	2
1:A:226:CYS:CB	1:A:232:PHE:CE1	0.68	2.77	8	4
1:A:216:VAL:HG23	1:A:225:TYR:HE1	0.67	1.49	5	18
1:A:164:CYS:HB2	1:A:173:THR:HG23	0.67	1.66	17	4
1:A:195:LEU:O	1:A:195:LEU:HD13	0.67	1.90	20	1
1:A:226:CYS:SG	1:A:234:LEU:HD13	0.67	2.30	7	10
1:A:216:VAL:HG12	1:A:216:VAL:O	0.67	1.89	15	9
1:A:224:CYS:O	1:A:234:LEU:HD13	0.67	1.90	1	4
1:A:205:GLU:O	1:A:210:MET:HG3	0.66	1.90	5	15
1:A:218:TYR:CE2	1:A:221:GLY:O	0.66	2.48	11	15
1:A:235:ALA:HB2	1:A:242:GLU:HB2	0.66	1.68	5	2
1:A:162:ASP:HB3	1:A:166:LEU:HD12	0.66	1.67	1	8
1:A:218:TYR:CD2	1:A:221:GLY:O	0.66	2.48	11	7
1:A:188:PRO:O	1:A:189:GLU:CG	0.66	2.44	3	6
1:A:170:ILE:CG2	1:A:183:PHE:CD2	0.65	2.80	18	15
1:A:187:CYS:HB3	1:A:191:TYR:HB2	0.65	1.67	20	10
1:A:167:LYS:HG3	1:A:170:ILE:HD11	0.65	1.67	7	2
1:A:216:VAL:O	1:A:216:VAL:HG12	0.65	1.91	13	9
1:A:174:ALA:HB2	1:A:193:TYR:CD1	0.65	2.27	11	1
1:A:187:CYS:HB2	1:A:191:TYR:O	0.64	1.91	7	2
1:A:197:SER:O	1:A:198:LYS:CD	0.64	2.46	2	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:ASN:HA	1:A:222:TYR:HA	0.64	1.70	17	20
1:A:175:VAL:O	1:A:175:VAL:HG12	0.63	1.92	2	10
1:A:179:ILE:HD11	1:A:182:ASP:HB3	0.63	1.70	4	20
1:A:216:VAL:O	1:A:223:THR:HB	0.63	1.94	15	8
1:A:214:LEU:N	1:A:214:LEU:HD22	0.63	2.09	12	9
1:A:208:GLU:O	1:A:209:ASN:CB	0.62	2.47	15	18
1:A:163:GLU:HA	1:A:178:ASN:CB	0.62	2.24	4	18
1:A:189:GLU:C	1:A:191:TYR:H	0.61	1.99	13	8
1:A:166:LEU:HD23	1:A:167:LYS:CG	0.61	2.25	11	1
1:A:190:GLY:O	1:A:203:ILE:CD1	0.61	2.49	15	19
1:A:237:ASP:O	1:A:238:GLN:CB	0.60	2.49	16	6
1:A:232:PHE:CB	1:A:243:VAL:HA	0.60	2.27	3	12
1:A:218:TYR:CE1	1:A:221:GLY:O	0.59	2.55	1	17
1:A:179:ILE:HD11	1:A:182:ASP:HB2	0.59	1.74	7	20
1:A:188:PRO:O	1:A:189:GLU:HB2	0.59	1.97	17	3
1:A:234:LEU:HD21	1:A:238:GLN:HA	0.58	1.75	4	2
1:A:230:LYS:HB3	1:A:232:PHE:CE2	0.58	2.33	14	1
1:A:203:ILE:O	3:A:249:HOH:O	0.58	2.21	15	1
1:A:234:LEU:HD12	1:A:235:ALA:N	0.58	2.13	12	4
1:A:201:GLU:O	1:A:202:ASP:O	0.58	2.21	14	12
1:A:218:TYR:CD1	1:A:221:GLY:O	0.58	2.57	6	17
1:A:216:VAL:CG2	1:A:225:TYR:CE1	0.58	2.87	14	15
1:A:223:THR:CG2	1:A:225:TYR:CZ	0.58	2.87	14	1
1:A:215:CYS:O	1:A:215:CYS:SG	0.58	2.62	17	10
1:A:235:ALA:HB2	1:A:242:GLU:CB	0.58	2.28	5	1
1:A:234:LEU:HD21	1:A:238:GLN:O	0.57	1.98	2	2
1:A:215:CYS:SG	1:A:215:CYS:O	0.57	2.63	4	5
1:A:170:ILE:HG22	1:A:171:CYS:N	0.57	2.15	16	4
1:A:233:LYS:O	1:A:242:GLU:O	0.56	2.23	2	12
1:A:214:LEU:HB3	1:A:225:TYR:CE1	0.56	2.35	5	11
1:A:214:LEU:CB	1:A:225:TYR:HB2	0.56	2.22	12	1
1:A:172:GLY:O	1:A:195:LEU:HD23	0.56	2.01	20	1
1:A:198:LYS:HD3	1:A:198:LYS:N	0.56	2.15	16	1
1:A:214:LEU:HD22	1:A:214:LEU:N	0.56	2.15	13	8
1:A:234:LEU:HD11	1:A:238:GLN:O	0.56	2.01	2	2
1:A:172:GLY:O	1:A:174:ALA:N	0.56	2.39	15	3
1:A:188:PRO:O	1:A:189:GLU:CB	0.56	2.54	3	9
1:A:188:PRO:O	1:A:191:TYR:HB2	0.55	2.01	16	6
1:A:218:TYR:HE2	1:A:223:THR:HG1	0.55	1.44	1	1
1:A:188:PRO:O	1:A:191:TYR:CD1	0.55	2.59	1	13
1:A:161:VAL:O	1:A:163:GLU:OE1	0.55	2.25	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:CYS:O	1:A:227:ASP:HB3	0.55	2.02	19	9
1:A:195:LEU:HD23	1:A:195:LEU:O	0.55	2.02	16	1
1:A:205:GLU:CB	1:A:222:TYR:CD1	0.55	2.90	1	13
1:A:213:GLN:O	1:A:214:LEU:HD22	0.55	2.01	1	1
1:A:183:PHE:CD1	1:A:183:PHE:C	0.55	2.80	20	8
1:A:183:PHE:C	1:A:183:PHE:CD1	0.54	2.79	1	9
1:A:174:ALA:HB2	1:A:193:TYR:CE1	0.54	2.38	11	1
1:A:205:GLU:HB2	1:A:222:TYR:HB3	0.54	1.79	12	13
1:A:194:ASN:O	1:A:198:LYS:N	0.54	2.40	5	10
1:A:226:CYS:O	1:A:227:ASP:C	0.54	2.45	5	5
1:A:208:GLU:O	1:A:209:ASN:HB2	0.54	2.03	9	2
1:A:175:VAL:HG12	1:A:175:VAL:O	0.53	2.03	10	6
1:A:212:ALA:O	1:A:214:LEU:N	0.53	2.42	9	5
1:A:205:GLU:OE2	1:A:220:GLY:O	0.53	2.26	7	16
1:A:235:ALA:HB3	1:A:237:ASP:OD1	0.53	2.04	18	1
1:A:187:CYS:HB3	1:A:191:TYR:CB	0.53	2.34	2	7
1:A:235:ALA:HB3	1:A:237:ASP:OD2	0.53	2.03	8	1
1:A:171:CYS:O	1:A:173:THR:N	0.53	2.41	15	2
1:A:217:ASN:HA	1:A:222:TYR:CA	0.53	2.34	12	9
1:A:234:LEU:HD13	1:A:240:SER:O	0.53	2.02	20	3
1:A:195:LEU:HD22	1:A:198:LYS:HD2	0.53	1.80	20	1
1:A:167:LYS:CE	1:A:170:ILE:HD11	0.52	2.35	15	1
1:A:225:TYR:N	1:A:225:TYR:CD1	0.52	2.78	14	1
1:A:227:ASP:HB3	1:A:232:PHE:O	0.52	2.05	14	4
1:A:166:LEU:HD23	1:A:167:LYS:HG3	0.52	1.80	11	1
1:A:191:TYR:CE1	1:A:220:GLY:HA2	0.52	2.40	4	6
1:A:214:LEU:CD2	1:A:226:CYS:O	0.51	2.58	1	2
1:A:164:CYS:SG	1:A:173:THR:HA	0.51	2.45	17	1
1:A:161:VAL:O	1:A:162:ASP:O	0.51	2.27	4	9
1:A:178:ASN:OD1	1:A:179:ILE:O	0.51	2.28	5	4
1:A:214:LEU:CB	1:A:225:TYR:CE2	0.51	2.94	10	11
1:A:218:TYR:CZ	1:A:221:GLY:O	0.51	2.64	3	20
1:A:234:LEU:HD11	1:A:238:GLN:HA	0.51	1.83	9	4
1:A:175:VAL:HG11	1:A:186:GLU:OE2	0.51	2.05	1	1
1:A:226:CYS:O	1:A:227:ASP:CG	0.51	2.49	20	2
1:A:226:CYS:O	1:A:227:ASP:OD1	0.50	2.29	18	1
1:A:170:ILE:CG2	1:A:183:PHE:CE2	0.50	2.95	1	4
1:A:232:PHE:CE2	1:A:241:CYS:HB3	0.50	2.41	13	1
1:A:216:VAL:O	1:A:216:VAL:CG1	0.50	2.59	15	4
1:A:189:GLU:HG3	1:A:191:TYR:CD1	0.50	2.41	2	1
1:A:187:CYS:CB	1:A:191:TYR:O	0.50	2.60	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:LYS:CB	1:A:232:PHE:CE2	0.50	2.95	1	2
1:A:170:ILE:HA	1:A:183:PHE:CE2	0.50	2.41	11	2
1:A:216:VAL:HB	1:A:225:TYR:CE1	0.50	2.41	14	1
1:A:227:ASP:OD1	1:A:227:ASP:O	0.50	2.29	13	2
1:A:192:ARG:O	1:A:201:GLU:O	0.50	2.30	10	9
1:A:163:GLU:O	1:A:178:ASN:ND2	0.50	2.45	20	4
1:A:197:SER:O	1:A:198:LYS:HD3	0.50	2.06	2	6
1:A:235:ALA:HB2	1:A:242:GLU:HG2	0.50	1.82	10	2
1:A:223:THR:HG21	1:A:225:TYR:CZ	0.50	2.41	14	1
1:A:227:ASP:HB2	1:A:232:PHE:O	0.50	2.07	3	4
1:A:212:ALA:HB1	1:A:226:CYS:SG	0.50	2.46	19	2
1:A:234:LEU:HD21	1:A:238:GLN:C	0.49	2.28	2	2
1:A:171:CYS:O	1:A:172:GLY:C	0.49	2.50	17	4
1:A:176:CYS:HA	1:A:184:GLU:O	0.49	2.07	15	8
1:A:205:GLU:HB3	1:A:222:TYR:CD1	0.49	2.42	3	16
1:A:167:LYS:CG	1:A:170:ILE:HD11	0.49	2.34	7	1
1:A:234:LEU:HD12	1:A:240:SER:O	0.49	2.07	1	3
1:A:214:LEU:HB3	1:A:225:TYR:CE2	0.49	2.43	13	12
1:A:188:PRO:C	1:A:189:GLU:CG	0.49	2.81	7	5
1:A:172:GLY:O	1:A:173:THR:C	0.49	2.50	11	11
1:A:188:PRO:O	1:A:189:GLU:C	0.49	2.49	1	6
1:A:237:ASP:O	1:A:238:GLN:HB3	0.49	2.08	19	1
1:A:191:TYR:CE1	1:A:220:GLY:CA	0.49	2.96	15	3
1:A:224:CYS:SG	1:A:239:LYS:HA	0.48	2.48	20	4
1:A:187:CYS:O	1:A:189:GLU:O	0.48	2.31	13	5
1:A:187:CYS:CB	1:A:191:TYR:HB2	0.48	2.38	2	3
1:A:191:TYR:CD1	1:A:202:ASP:HA	0.48	2.43	2	3
1:A:203:ILE:HG23	1:A:205:GLU:CG	0.48	2.36	18	4
1:A:224:CYS:O	1:A:234:LEU:HD22	0.48	2.07	11	1
1:A:226:CYS:SG	1:A:232:PHE:CE2	0.48	3.07	18	3
1:A:176:CYS:HA	1:A:185:CYS:HB3	0.47	1.85	17	1
1:A:213:GLN:HB3	1:A:214:LEU:HD22	0.47	1.86	18	2
1:A:189:GLU:C	1:A:191:TYR:N	0.47	2.67	6	6
1:A:171:CYS:HB3	1:A:176:CYS:SG	0.47	2.49	15	3
1:A:234:LEU:O	1:A:235:ALA:O	0.47	2.33	4	7
1:A:216:VAL:CG1	1:A:216:VAL:O	0.47	2.61	2	3
1:A:211:CYS:HB2	1:A:215:CYS:HB3	0.47	1.86	17	12
1:A:214:LEU:O	1:A:224:CYS:HA	0.47	2.09	10	2
1:A:203:ILE:HG23	1:A:205:GLU:OE1	0.47	2.09	10	4
1:A:203:ILE:HG22	3:A:249:HOH:O	0.47	2.09	4	1
1:A:227:ASP:OD1	1:A:232:PHE:N	0.47	2.48	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:232:PHE:HE2	1:A:241:CYS:HB3	0.47	1.70	15	8
1:A:205:GLU:O	1:A:210:MET:CG	0.47	2.63	6	6
1:A:203:ILE:CG2	1:A:205:GLU:HG3	0.47	2.37	5	4
1:A:240:SER:O	1:A:241:CYS:SG	0.47	2.73	3	2
1:A:213:GLN:CB	1:A:226:CYS:HA	0.47	2.40	17	4
1:A:237:ASP:O	1:A:238:GLN:HB2	0.46	2.10	17	2
1:A:189:GLU:CG	1:A:191:TYR:CD1	0.46	2.98	2	1
1:A:201:GLU:O	1:A:202:ASP:C	0.46	2.54	16	14
1:A:162:ASP:O	1:A:166:LEU:CD1	0.46	2.63	17	1
1:A:193:TYR:OH	1:A:198:LYS:C	0.46	2.54	14	3
1:A:205:GLU:HB2	1:A:222:TYR:CD1	0.46	2.46	5	2
1:A:164:CYS:CB	1:A:173:THR:HA	0.46	2.40	15	3
1:A:205:GLU:HB3	1:A:222:TYR:CG	0.46	2.45	12	1
1:A:189:GLU:HB2	1:A:191:TYR:CD1	0.46	2.45	3	1
1:A:193:TYR:CD2	1:A:199:SER:O	0.46	2.68	1	4
1:A:230:LYS:HB2	1:A:232:PHE:CE2	0.46	2.45	3	2
1:A:234:LEU:HD11	1:A:238:GLN:CA	0.46	2.41	4	2
1:A:234:LEU:HD11	1:A:237:ASP:O	0.46	2.11	20	1
1:A:187:CYS:CB	1:A:191:TYR:CB	0.46	2.93	2	1
1:A:183:PHE:O	1:A:183:PHE:CD1	0.46	2.69	5	4
1:A:218:TYR:CG	1:A:221:GLY:O	0.46	2.70	15	20
1:A:216:VAL:HG23	1:A:225:TYR:CZ	0.46	2.44	8	2
1:A:195:LEU:O	1:A:198:LYS:CD	0.46	2.64	10	10
1:A:183:PHE:CE2	1:A:185:CYS:SG	0.45	3.09	10	2
1:A:205:GLU:CB	1:A:222:TYR:CG	0.45	2.99	12	1
1:A:179:ILE:CD1	1:A:182:ASP:CB	0.45	2.94	16	12
1:A:224:CYS:O	1:A:234:LEU:HD11	0.45	2.11	5	1
1:A:234:LEU:CD1	1:A:240:SER:O	0.45	2.65	14	6
1:A:191:TYR:CZ	1:A:220:GLY:CA	0.45	3.00	4	3
1:A:224:CYS:O	1:A:234:LEU:HD12	0.45	2.11	2	1
1:A:226:CYS:O	1:A:227:ASP:CB	0.45	2.65	19	2
1:A:191:TYR:CD2	1:A:202:ASP:N	0.45	2.84	16	2
1:A:188:PRO:O	1:A:191:TYR:CB	0.45	2.65	16	3
1:A:195:LEU:O	1:A:198:LYS:HD3	0.45	2.11	17	5
1:A:214:LEU:CB	1:A:225:TYR:O	0.45	2.59	11	1
1:A:214:LEU:CD2	1:A:214:LEU:N	0.45	2.80	12	2
1:A:213:GLN:HB2	1:A:226:CYS:SG	0.45	2.52	18	2
1:A:183:PHE:CD1	1:A:183:PHE:O	0.44	2.69	12	5
1:A:216:VAL:CB	1:A:225:TYR:HE1	0.44	2.25	14	1
1:A:205:GLU:OE2	1:A:222:TYR:N	0.44	2.50	19	2
1:A:198:LYS:CD	1:A:198:LYS:N	0.44	2.80	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ILE:O	1:A:217:ASN:ND2	0.44	2.50	17	2
1:A:232:PHE:HB3	1:A:243:VAL:HG23	0.44	1.88	12	10
1:A:206:CYS:SG	1:A:215:CYS:O	0.44	2.75	14	2
1:A:226:CYS:SG	1:A:234:LEU:HA	0.44	2.52	2	2
1:A:167:LYS:HE2	1:A:170:ILE:HD11	0.44	1.88	7	2
1:A:188:PRO:O	1:A:189:GLU:HB3	0.44	2.13	2	1
1:A:225:TYR:HA	1:A:234:LEU:HB2	0.43	1.90	14	2
1:A:224:CYS:O	1:A:238:GLN:O	0.43	2.36	14	1
1:A:190:GLY:O	1:A:203:ILE:CB	0.43	2.65	9	1
1:A:211:CYS:HB3	1:A:214:LEU:O	0.43	2.12	12	1
1:A:206:CYS:HB3	1:A:217:ASN:HB2	0.43	1.90	6	1
1:A:195:LEU:O	1:A:198:LYS:HD2	0.43	2.12	16	2
1:A:167:LYS:CB	1:A:170:ILE:HD11	0.43	2.41	10	1
1:A:213:GLN:HG3	1:A:214:LEU:CD2	0.43	2.43	9	2
1:A:176:CYS:CB	1:A:184:GLU:O	0.43	2.66	1	1
1:A:232:PHE:HB2	1:A:243:VAL:CA	0.43	2.39	13	4
1:A:191:TYR:CG	1:A:202:ASP:HA	0.43	2.49	19	1
1:A:205:GLU:OE1	1:A:222:TYR:N	0.43	2.51	2	1
1:A:224:CYS:O	1:A:234:LEU:CD1	0.43	2.66	5	1
1:A:214:LEU:HD12	1:A:225:TYR:CE2	0.43	2.49	8	1
1:A:206:CYS:HB2	1:A:215:CYS:HB2	0.43	1.53	15	4
1:A:193:TYR:OH	1:A:198:LYS:CA	0.43	2.67	10	2
1:A:211:CYS:CB	1:A:215:CYS:HB3	0.43	2.44	11	3
1:A:163:GLU:HA	1:A:178:ASN:HB3	0.43	1.90	2	4
1:A:205:GLU:OE1	1:A:217:ASN:ND2	0.43	2.52	17	2
1:A:191:TYR:CD2	1:A:202:ASP:HA	0.43	2.49	6	3
1:A:216:VAL:CB	1:A:225:TYR:CE1	0.43	3.02	14	1
1:A:187:CYS:O	1:A:188:PRO:C	0.43	2.56	19	5
1:A:226:CYS:O	1:A:227:ASP:OD2	0.43	2.37	13	1
1:A:205:GLU:OE1	1:A:220:GLY:O	0.43	2.37	2	1
1:A:163:GLU:O	1:A:178:ASN:HB2	0.42	2.14	20	1
1:A:227:ASP:CB	1:A:232:PHE:O	0.42	2.67	13	1
1:A:178:ASN:ND2	1:A:182:ASP:O	0.42	2.52	7	3
1:A:225:TYR:CB	1:A:234:LEU:HB2	0.42	2.44	1	1
1:A:211:CYS:HB2	1:A:215:CYS:CB	0.42	2.43	9	1
1:A:193:TYR:CD1	1:A:199:SER:O	0.42	2.72	18	1
1:A:226:CYS:HB2	1:A:241:CYS:HB2	0.42	1.72	5	2
1:A:178:ASN:OD1	1:A:179:ILE:N	0.42	2.53	6	1
1:A:161:VAL:HG22	1:A:162:ASP:N	0.42	2.30	8	1
1:A:187:CYS:O	1:A:188:PRO:O	0.42	2.38	11	2
1:A:205:GLU:H	1:A:217:ASN:ND2	0.42	2.12	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:GLU:O	1:A:209:ASN:C	0.42	2.58	2	1
1:A:211:CYS:SG	1:A:215:CYS:CB	0.42	3.08	6	2
1:A:216:VAL:HB	1:A:225:TYR:HE1	0.42	1.74	14	1
1:A:170:ILE:HG22	1:A:183:PHE:CE2	0.42	2.50	12	1
1:A:164:CYS:SG	1:A:171:CYS:CB	0.42	3.08	6	1
1:A:226:CYS:CB	1:A:232:PHE:HE1	0.41	2.27	1	1
1:A:234:LEU:HD23	1:A:240:SER:O	0.41	2.14	5	1
1:A:227:ASP:O	1:A:227:ASP:CG	0.41	2.59	18	1
1:A:214:LEU:CB	1:A:225:TYR:CZ	0.41	2.99	17	2
1:A:213:GLN:HB3	1:A:214:LEU:CD2	0.41	2.45	18	1
1:A:171:CYS:O	1:A:171:CYS:SG	0.41	2.78	7	1
1:A:214:LEU:N	1:A:214:LEU:CD2	0.41	2.82	13	5
1:A:175:VAL:HG21	1:A:186:GLU:HG3	0.41	1.92	4	1
1:A:213:GLN:CG	1:A:226:CYS:HA	0.41	2.46	9	1
1:A:164:CYS:HB2	1:A:173:THR:HG22	0.41	1.91	13	1
1:A:161:VAL:O	1:A:162:ASP:C	0.41	2.59	12	1
1:A:170:ILE:HG23	1:A:183:PHE:HD2	0.41	1.74	17	1
1:A:162:ASP:CB	1:A:166:LEU:CD1	0.41	2.99	16	1
1:A:163:GLU:CA	1:A:178:ASN:HB3	0.41	2.45	16	1
1:A:216:VAL:HG23	1:A:225:TYR:OH	0.41	2.16	16	1
1:A:230:LYS:HB2	1:A:232:PHE:CD2	0.41	2.51	3	1
1:A:217:ASN:CG	1:A:222:TYR:HB3	0.41	2.35	1	1
1:A:170:ILE:CG2	1:A:171:CYS:N	0.41	2.83	15	2
1:A:205:GLU:HB2	1:A:222:TYR:CB	0.41	2.46	12	1
1:A:192:ARG:N	1:A:201:GLU:O	0.41	2.54	17	2
1:A:202:ASP:CB	1:A:219:PRO:HA	0.41	2.46	17	1
1:A:161:VAL:HG12	1:A:162:ASP:N	0.41	2.31	14	1
1:A:203:ILE:CG2	1:A:205:GLU:CD	0.41	2.90	16	1
1:A:230:LYS:HB3	1:A:232:PHE:CD2	0.40	2.51	1	1
1:A:213:GLN:OE1	1:A:232:PHE:CE1	0.40	2.74	18	1
1:A:235:ALA:HB3	1:A:240:SER:OG	0.40	2.16	3	1
1:A:164:CYS:SG	1:A:171:CYS:HB3	0.40	2.56	9	1
1:A:163:GLU:CB	1:A:178:ASN:HB3	0.40	2.46	12	1
1:A:196:LYS:CD	1:A:196:LYS:N	0.40	2.85	5	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	84/87 (97%)	54±2 (64±3%)	19±3 (22±3%)	11±1 (13±2%)	1	6
All	All	1680/1740 (97%)	1080 (64%)	377 (22%)	223 (13%)	1	6

All 21 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	219	PRO	20
1	A	188	PRO	20
1	A	162	ASP	20
1	A	235	ALA	20
1	A	209	ASN	19
1	A	189	GLU	18
1	A	202	ASP	17
1	A	175	VAL	14
1	A	173	THR	12
1	A	228	GLY	9
1	A	227	ASP	9
1	A	238	GLN	7
1	A	190	GLY	7
1	A	172	GLY	6
1	A	213	GLN	6
1	A	160	ASP	5
1	A	170	ILE	4
1	A	212	ALA	3
1	A	237	ASP	3
1	A	174	ALA	3
1	A	226	CYS	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	74/77 (96%)	51±2 (69±3%)	23±2 (31±3%)	1	14
All	All	1480/1540 (96%)	1016 (69%)	464 (31%)	1	14

All 52 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	160	ASP	20
1	A	182	ASP	20
1	A	198	LYS	19
1	A	173	THR	19
1	A	183	PHE	18
1	A	171	CYS	18
1	A	196	LYS	17
1	A	237	ASP	15
1	A	240	SER	15
1	A	210	MET	13
1	A	206	CYS	13
1	A	207	SER	13
1	A	229	LYS	13
1	A	239	LYS	12
1	A	166	LEU	12
1	A	204	ASP	12
1	A	187	CYS	11
1	A	177	LYS	11
1	A	176	CYS	11
1	A	236	GLN	11
1	A	226	CYS	10
1	A	230	LYS	9
1	A	186	GLU	9
1	A	233	LYS	9
1	A	189	GLU	8
1	A	195	LEU	8
1	A	238	GLN	7
1	A	165	SER	7
1	A	185	CYS	7
1	A	194	ASN	7
1	A	167	LYS	7
1	A	164	CYS	6
1	A	213	GLN	6
1	A	197	SER	6
1	A	170	ILE	6
1	A	201	GLU	6
1	A	202	ASP	6
1	A	205	GLU	6
1	A	163	GLU	5
1	A	227	ASP	4
1	A	224	CYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	209	ASN	4
1	A	199	SER	4
1	A	234	LEU	4
1	A	162	ASP	3
1	A	192	ARG	3
1	A	208	GLU	3
1	A	242	GLU	2
1	A	225	TYR	2
1	A	169	SER	1
1	A	200	CYS	1
1	A	184	GLU	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 2 ligands modelled in this entry, 2 are 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