



Full wwPDB NMR Structure Validation Report ⓘ

Mar 30, 2026 – 10:01 AM UTC

PDB ID : 1Z6C / pdb_00001z6c
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

<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

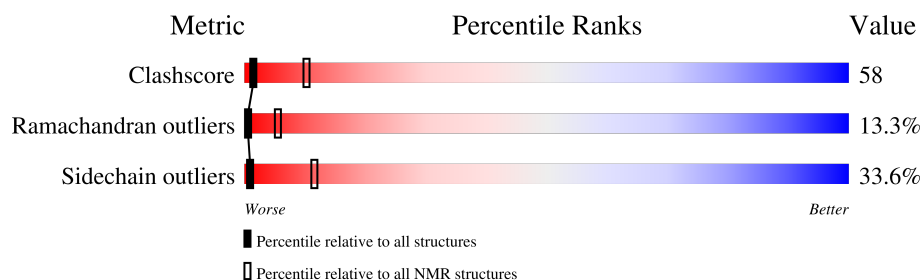
1 Overall quality at a glance

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	87	18% 54% 24% .

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)	1.05	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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is water.

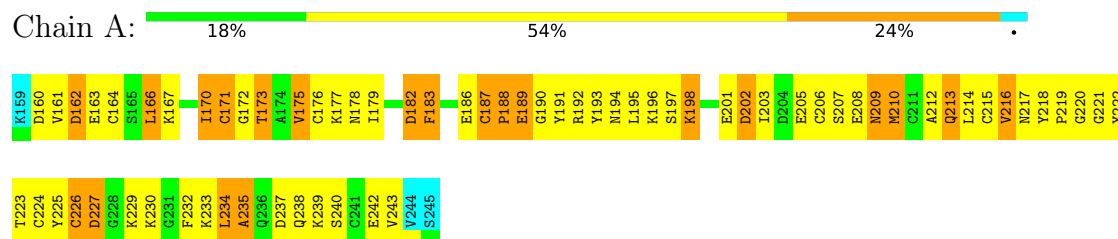
Mol	Chain	Residues	Atoms		
3	A	2	Total	H	O
			6	4	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: Vitamin K-dependent protein S

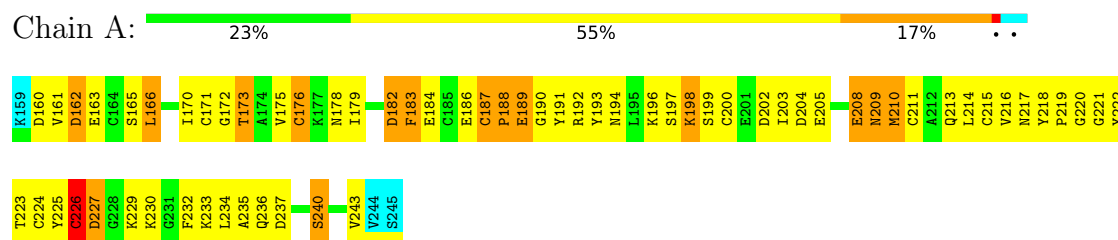


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

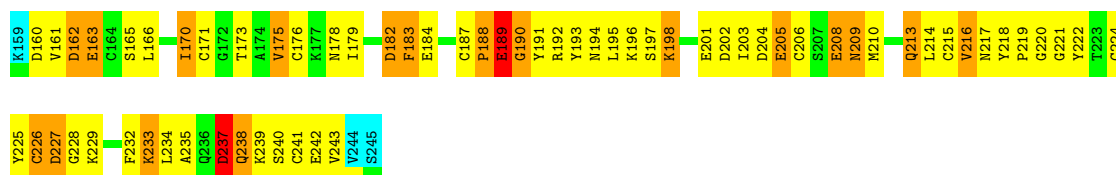
- Molecule 1: Vitamin K-dependent protein S



4.2.2 Score per residue for model 2

- Molecule 1: Vitamin K-dependent protein S

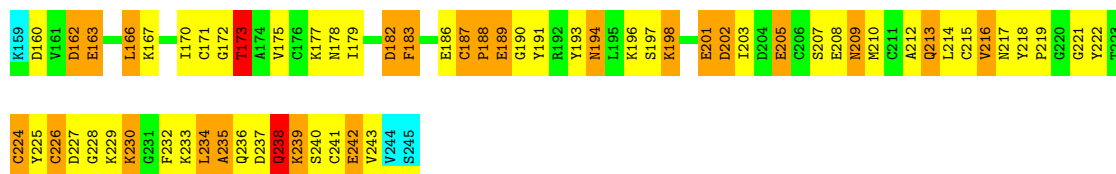




4.2.3 Score per residue for model 3

- Molecule 1: Vitamin K-dependent protein S

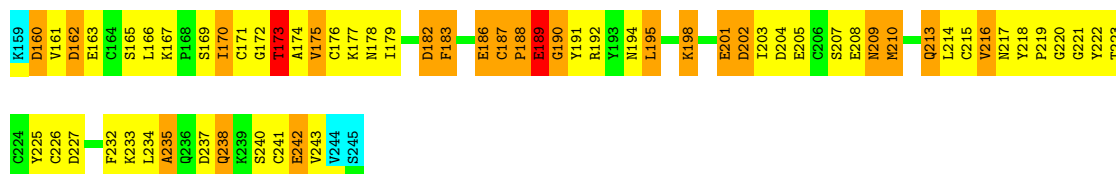
Chain A: 24% 44% 26% . .



4.2.4 Score per residue for model 4

- Molecule 1: Vitamin K-dependent protein S

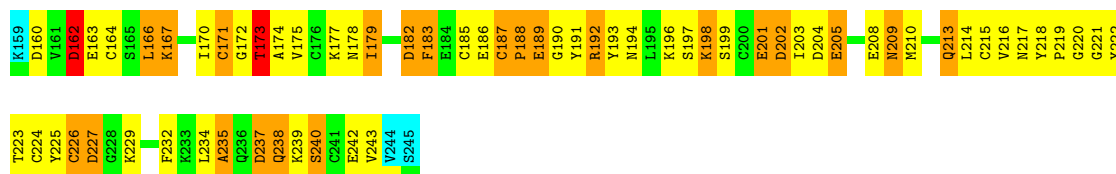
Chain A: 24% 46% 24% . .



4.2.5 Score per residue for model 5

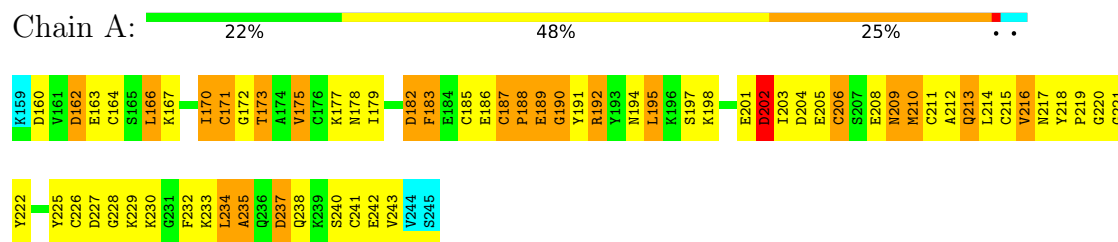
- Molecule 1: Vitamin K-dependent protein S

Chain A: 23% 46% 25% . .



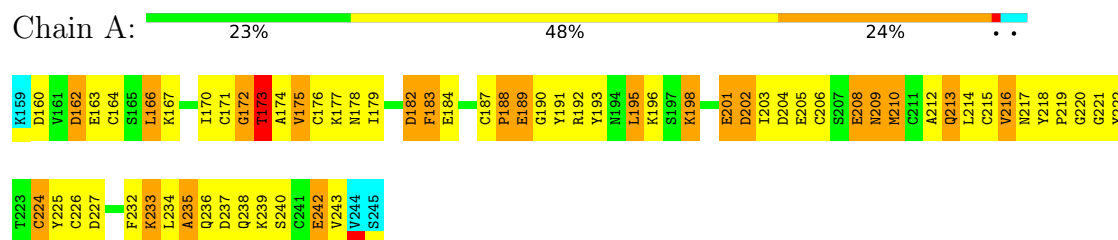
4.2.6 Score per residue for model 6

- Molecule 1: Vitamin K-dependent protein S



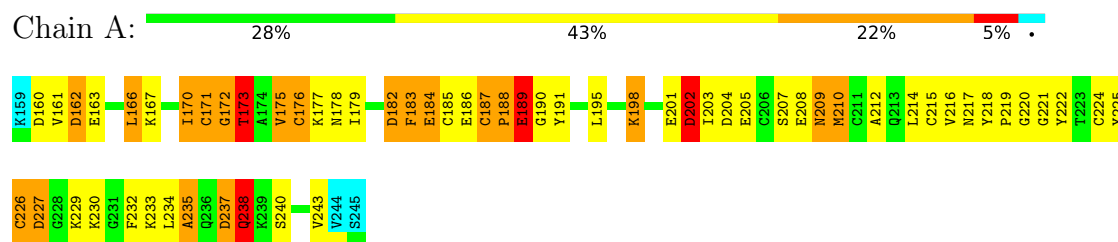
4.2.7 Score per residue for model 7

- Molecule 1: Vitamin K-dependent protein S



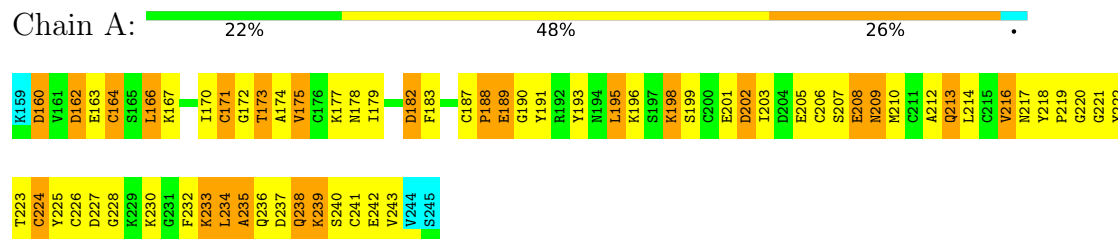
4.2.8 Score per residue for model 8

- Molecule 1: Vitamin K-dependent protein S



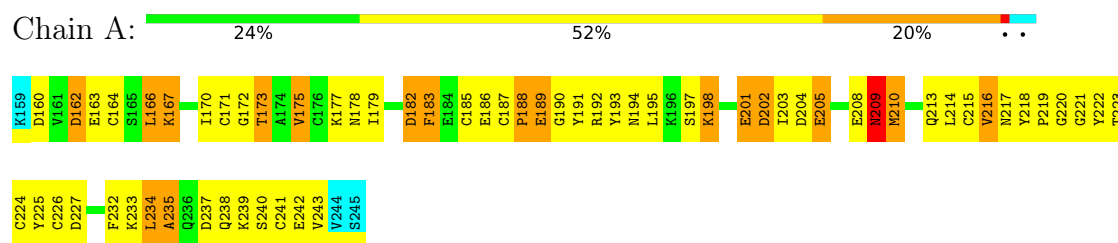
4.2.9 Score per residue for model 9

- Molecule 1: Vitamin K-dependent protein S



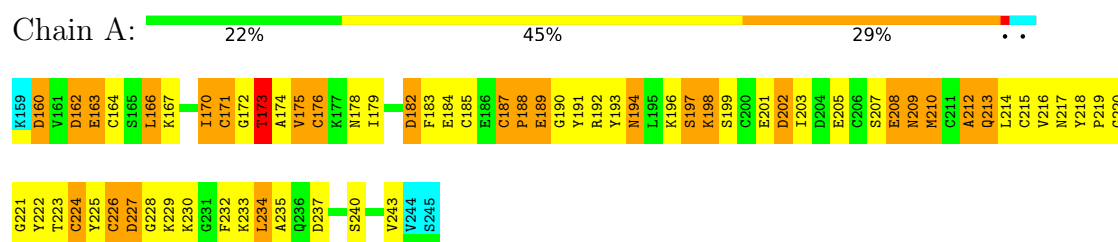
4.2.10 Score per residue for model 10

- Molecule 1: Vitamin K-dependent protein S



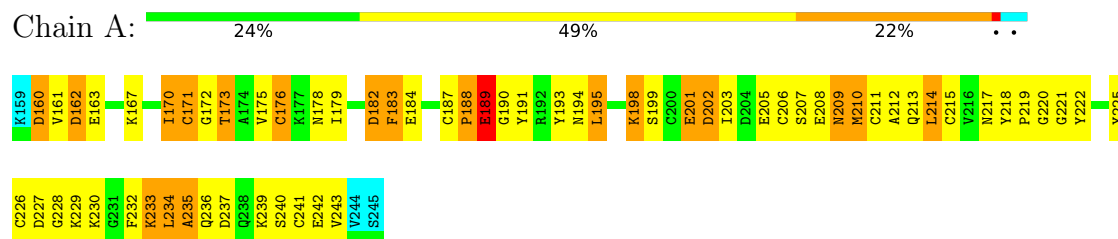
4.2.11 Score per residue for model 11

- Molecule 1: Vitamin K-dependent protein S



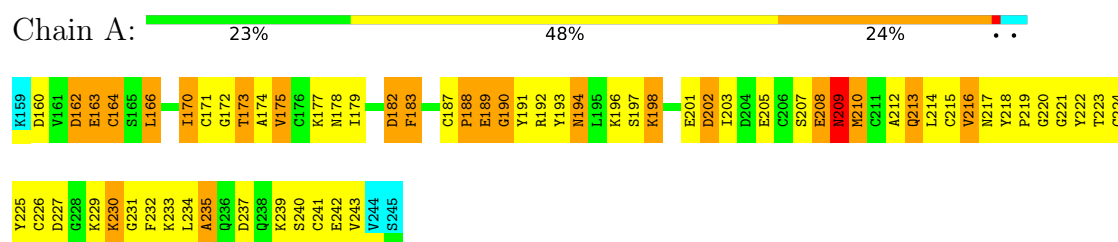
4.2.12 Score per residue for model 12

- Molecule 1: Vitamin K-dependent protein S



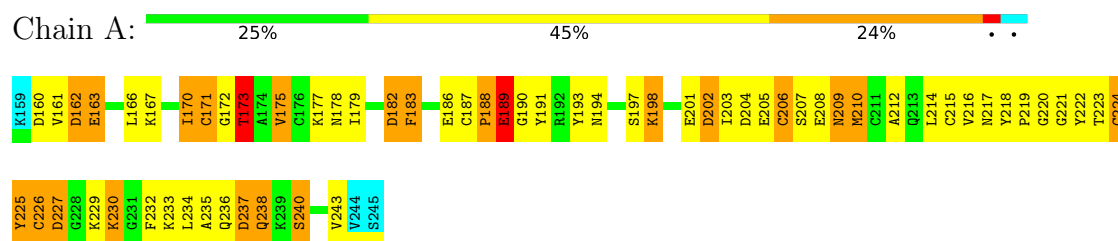
4.2.13 Score per residue for model 13

- Molecule 1: Vitamin K-dependent protein S



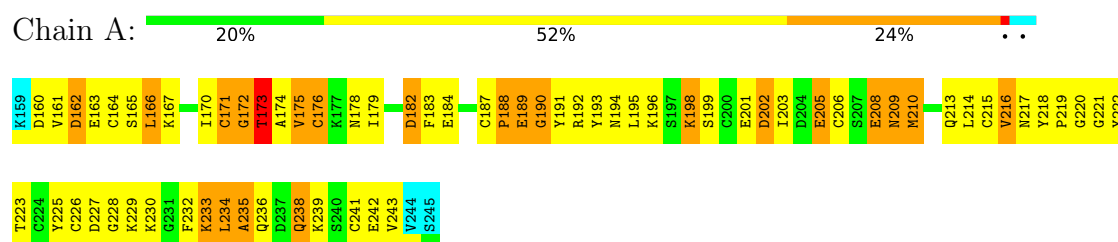
4.2.14 Score per residue for model 14

- Molecule 1: Vitamin K-dependent protein S



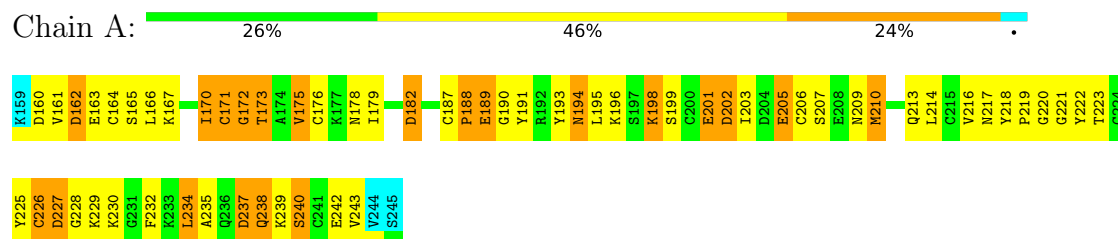
4.2.15 Score per residue for model 15

- Molecule 1: Vitamin K-dependent protein S



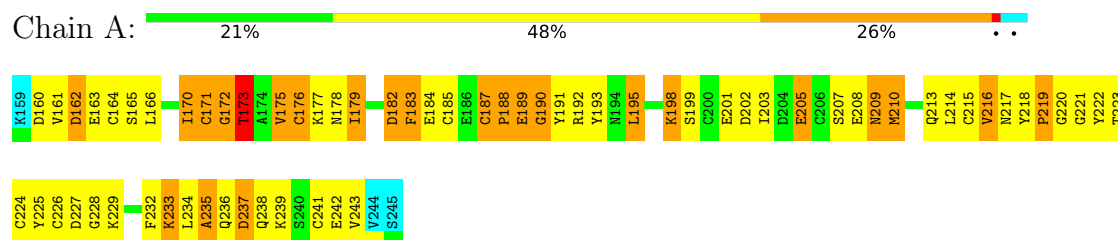
4.2.16 Score per residue for model 16

- Molecule 1: Vitamin K-dependent protein S



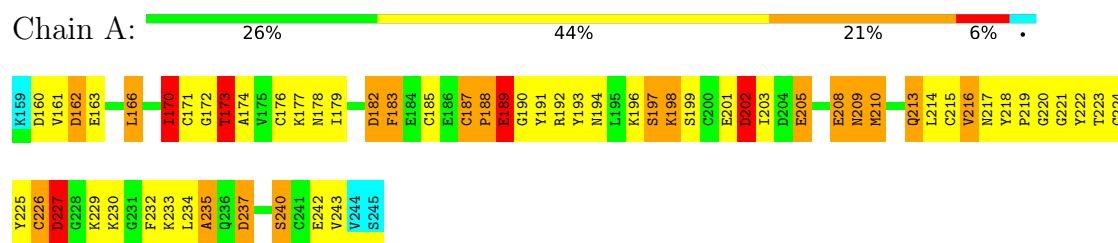
4.2.17 Score per residue for model 17

- Molecule 1: Vitamin K-dependent protein S



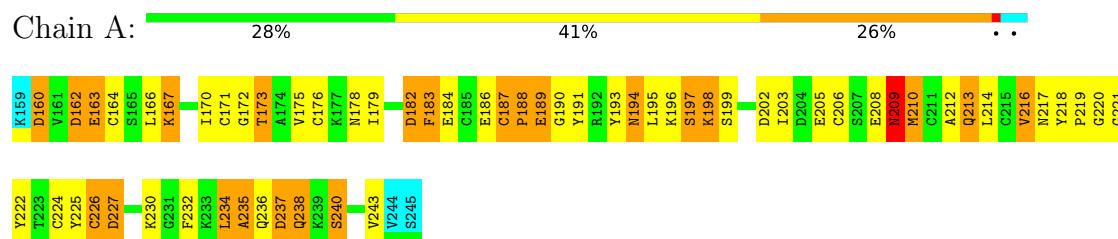
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Vitamin K-dependent protein S



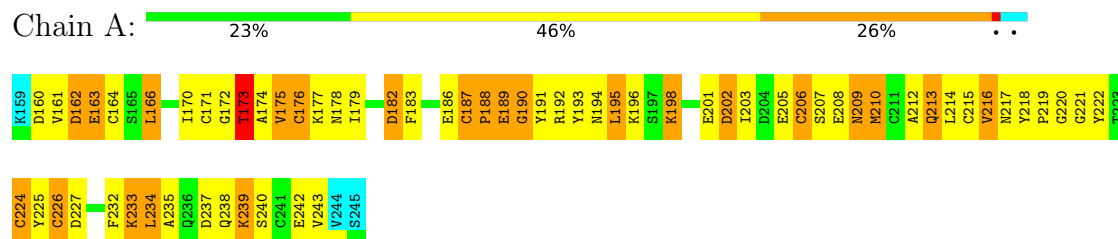
4.2.19 Score per residue for model 19

- 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.

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	71±4
3	A	2	4	0	1±1
All	All	12820	11720	11640	1418

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 58.

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:213:GLN:C	1:A:214:LEU:HD22	0.80	2.01	6	16
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: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:216:VAL:HG12	1:A:216:VAL:O	0.67	1.89	15	18
1:A:226:CYS:SG	1:A:234:LEU:HD13	0.67	2.30	7	10
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:162:ASP:HB3	1:A:166:LEU:HD12	0.66	1.67	1	8
1:A:189:GLU:C	1:A:191:TYR:H	0.66	1.99	13	8
1:A:235:ALA:HB2	1:A:242:GLU:HB2	0.66	1.68	5	2
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: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	15	20
1:A:175:VAL:HG12	1:A:175:VAL:O	0.63	1.92	2	14
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:HD22	1:A:214:LEU:N	0.63	2.09	12	17
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: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:183:PHE:C	1:A:183:PHE:CD1	0.59	2.80	9	15
1:A:188:PRO:O	1:A:189:GLU:HB2	0.59	1.97	17	3
1:A:226:CYS:O	1:A:227:ASP:C	0.59	2.45	5	5
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:SG	1:A:215:CYS:O	0.58	2.62	17	14
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:170:ILE:HG22	1:A:171:CYS:N	0.57	2.15	16	4
1:A:214:LEU:HB3	1:A:225:TYR:CE1	0.56	2.35	5	11
1:A:233:LYS:O	1:A:242:GLU:O	0.56	2.23	2	12
1:A:214:LEU:CB	1:A:225:TYR:HB2	0.56	2.22	12	1
1:A:198:LYS:N	1:A:198:LYS:HD3	0.56	2.15	16	1
1:A:172:GLY:O	1:A:195:LEU:HD23	0.56	2.01	20	1
1:A:234:LEU:HD11	1:A:238:GLN:O	0.56	2.01	2	2
1:A:188:PRO:O	1:A:189:GLU:CB	0.56	2.54	3	9
1:A:172:GLY:O	1:A:174:ALA:N	0.56	2.39	15	3
1:A:188:PRO:O	1:A:191:TYR:HB2	0.55	2.01	16	6
1:A:188:PRO:O	1:A:191:TYR:CD1	0.55	2.59	1	13
1:A:226:CYS:O	1:A:227:ASP:CG	0.55	2.49	20	3
1:A:161:VAL:O	1:A:163:GLU:OE1	0.55	2.25	12	1
1:A:226:CYS:O	1:A:227:ASP:HB3	0.55	2.02	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:LEU:O	1:A:195:LEU:HD23	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:174:ALA:HB2	1:A:193:TYR:CE1	0.54	2.38	11	1
1:A:171:CYS:O	1:A:172:GLY:C	0.54	2.50	17	7
1:A:194:ASN:O	1:A:198:LYS:N	0.54	2.40	5	10
1:A:205:GLU:HB2	1:A:222:TYR:HB3	0.54	1.79	12	13
1:A:208:GLU:O	1:A:209:ASN:HB2	0.54	2.03	9	2
1:A:234:LEU:HD21	1:A:238:GLN:C	0.54	2.28	2	2
1:A:188:PRO:C	1:A:189:GLU:CG	0.53	2.80	9	7
1:A:172:GLY:O	1:A:173:THR:C	0.53	2.50	11	18
1:A:188:PRO:O	1:A:189:GLU:C	0.53	2.49	1	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:171:CYS:O	1:A:173:THR:N	0.53	2.41	15	2
1:A:235:ALA:HB3	1:A:237:ASP:OD2	0.53	2.03	8	1
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:189:GLU:C	1:A:191:TYR:N	0.52	2.67	6	6
1:A:167:LYS:CE	1:A:170:ILE:HD11	0.52	2.35	15	1
1:A:225:TYR:CD1	1:A:225:TYR:N	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	6	11
1:A:201:GLU:O	1:A:202:ASP:C	0.51	2.54	16	16
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:193:TYR:OH	1:A:198:LYS:C	0.51	2.54	14	11
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:189:GLU:HG3	1:A:191:TYR:CD1	0.50	2.41	2	1

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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:187:CYS:CB	1:A:191:TYR:O	0.50	2.60	14	7
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:197:SER:O	1:A:198:LYS:HD3	0.50	2.06	2	6
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: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: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:191:TYR:CE1	1:A:220:GLY:CA	0.49	2.96	15	3
1:A:237:ASP:O	1:A:238:GLN:HB3	0.49	2.08	19	1
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:187:CYS:O	1:A:188:PRO:C	0.47	2.56	19	6
1:A:213:GLN:HB3	1:A:214:LEU:HD22	0.47	1.86	18	2
1:A:176:CYS:HA	1:A:185:CYS:HB3	0.47	1.85	17	1
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:O	1:A:216:VAL:CG1	0.47	2.61	2	2
1:A:214:LEU:O	1:A:224:CYS:HA	0.47	2.09	10	2
1:A:203:ILE:HG22	3:A:249:HOH:O	0.47	2.09	4	1
1:A:203:ILE:HG23	1:A:205:GLU:OE1	0.47	2.09	10	4
1:A:227:ASP:OD1	1:A:232:PHE:N	0.47	2.48	16	1
1:A:205:GLU:O	1:A:210:MET:CG	0.47	2.63	6	6
1:A:232:PHE:HE2	1:A:241:CYS:HB3	0.47	1.70	15	8
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:GLU:CG	1:A:191:TYR:CD1	0.46	2.98	2	1
1:A:208:GLU:O	1:A:209:ASN:C	0.46	2.58	2	1
1:A:237:ASP:O	1:A:238:GLN:HB2	0.46	2.10	17	2
1:A:162:ASP:O	1:A:166:LEU:CD1	0.46	2.63	17	1
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:227:ASP:O	1:A:227:ASP:CG	0.46	2.59	18	1
1:A:193:TYR:CD2	1:A:199:SER:O	0.46	2.68	1	4
1:A:189:GLU:HB2	1:A:191:TYR:CD1	0.46	2.45	3	1
1:A:230:LYS:HB2	1:A:232:PHE:CE2	0.46	2.45	3	2
1:A:187:CYS:CB	1:A:191:TYR:CB	0.46	2.93	2	1
1:A:234:LEU:HD11	1:A:238:GLN:CA	0.46	2.41	4	2
1:A:161:VAL:O	1:A:162:ASP:C	0.46	2.59	12	1
1:A:234:LEU:HD11	1:A:237:ASP:O	0.46	2.11	20	1
1:A:217:ASN:CG	1:A:222:TYR:HB3	0.46	2.35	1	5
1:A:183:PHE:CD1	1:A:183:PHE:O	0.46	2.69	5	9
1:A:183:PHE:CD1	1:A:183:PHE:C	0.46	2.93	18	3
1:A:218:TYR:CG	1:A:221:GLY:O	0.46	2.70	15	20
1:A:195:LEU:O	1:A:198:LYS:CD	0.46	2.64	10	10
1:A:216:VAL:HG23	1:A:225:TYR:CZ	0.46	2.44	8	2
1:A:183:PHE:CE2	1:A:185:CYS:SG	0.45	3.09	10	2
1:A:203:ILE:CG2	1:A:205:GLU:CD	0.45	2.90	16	6
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:224:CYS:O	1:A:234:LEU:HD12	0.45	2.11	2	1
1:A:191:TYR:CZ	1:A:220:GLY:CA	0.45	3.00	4	3
1:A:191:TYR:CD2	1:A:202:ASP:N	0.45	2.84	16	2
1:A:226:CYS:O	1:A:227:ASP:CB	0.45	2.65	19	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:N	1:A:214:LEU:CD2	0.45	2.80	12	7
1:A:227:ASP:CG	1:A:232:PHE:O	0.45	2.59	19	4
1:A:213:GLN:HB2	1:A:226:CYS:SG	0.45	2.52	18	2
1:A:216:VAL:CB	1:A:225:TYR:HE1	0.44	2.25	14	1
1:A:236:GLN:O	1:A:237:ASP:C	0.44	2.59	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:227:ASP:HB2	1:A:232:PHE:C	0.44	2.38	16	1
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:234:LEU:HD12	1:A:234:LEU:C	0.44	2.37	12	4
1:A:188:PRO:O	1:A:189:GLU:HB3	0.44	2.13	2	1
1:A:167:LYS:HE2	1:A:170:ILE:HD11	0.44	1.88	7	2
1:A:225:TYR:HA	1:A:234:LEU:HB2	0.43	1.90	14	2
1:A:195:LEU:O	1:A:198:LYS:HD2	0.43	2.12	16	2
1:A:206:CYS:HB3	1:A:217:ASN:HB2	0.43	1.90	6	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:224:CYS:O	1:A:238:GLN:O	0.43	2.36	14	1
1:A:197:SER:C	1:A:198:LYS:CD	0.43	2.91	18	1
1:A:213:GLN:HG3	1:A:214:LEU:CD2	0.43	2.43	9	2
1:A:167:LYS:CB	1:A:170:ILE:HD11	0.43	2.41	10	1
1:A:176:CYS:CB	1:A:184:GLU:O	0.43	2.66	1	1
1:A:205:GLU:OE1	1:A:222:TYR:N	0.43	2.51	2	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: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:193:TYR:OH	1:A:198:LYS:CA	0.43	2.67	10	2
1:A:197:SER:C	1:A:198:LYS:CG	0.43	2.92	2	6
1:A:163:GLU:HA	1:A:178:ASN:HB3	0.43	1.90	2	4
1:A:191:TYR:CD2	1:A:202:ASP:HA	0.43	2.49	6	3
1:A:205:GLU:OE1	1:A:217:ASN:ND2	0.43	2.52	17	2
1:A:216:VAL:CB	1:A:225:TYR:CE1	0.43	3.02	14	1
1:A:226:CYS:O	1:A:227:ASP:OD2	0.43	2.37	13	1
1:A:234:LEU:C	1:A:234:LEU:HD12	0.43	2.39	20	1
1:A:205:GLU:OE1	1:A:220:GLY:O	0.43	2.37	2	1
1:A:227:ASP:CB	1:A:232:PHE:O	0.42	2.67	13	1
1:A:163:GLU:O	1:A:178:ASN:HB2	0.42	2.14	20	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:193:TYR:CD1	1:A:199:SER:O	0.42	2.72	18	1
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:211:CYS:SG	1:A:215:CYS:CB	0.42	3.08	6	2
1:A:175:VAL:O	1:A:175:VAL:HG12	0.42	2.15	5	2
1:A:164:CYS:SG	1:A:171:CYS:CB	0.42	3.08	6	1
1:A:170:ILE:HG22	1:A:183:PHE:CE2	0.42	2.50	12	1
1:A:216:VAL:HB	1:A:225:TYR:HE1	0.42	1.74	14	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:212:ALA:O	1:A:213:GLN:C	0.41	2.63	19	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: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:193:TYR:CE1	1:A:199:SER:C	0.41	2.99	16	1
1:A:164:CYS:HB2	1:A:173:THR:HG22	0.41	1.91	13	1
1:A:170:ILE:HG23	1:A:183:PHE:HD2	0.41	1.74	17	1
1:A:190:GLY:O	1:A:191:TYR:C	0.41	2.64	7	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:205:GLU:HB2	1:A:222:TYR:CB	0.41	2.46	12	1
1:A:230:LYS:O	1:A:231:GLY:C	0.41	2.63	13	1
1:A:170:ILE:CG2	1:A:171:CYS:N	0.41	2.83	15	2
1:A:171:CYS:C	1:A:193:TYR:HB3	0.41	2.41	16	2
1:A:192:ARG:N	1:A:201:GLU:O	0.41	2.54	2	2
1:A:161:VAL:HG12	1:A:162:ASP:N	0.41	2.31	14	1
1:A:202:ASP:CB	1:A:219:PRO:HA	0.41	2.46	17	1
1:A:230:LYS:HB3	1:A:232:PHE:CD2	0.40	2.51	1	1
1:A:215:CYS:O	1:A:215:CYS:SG	0.40	2.79	15	1
1:A:213:GLN:OE1	1:A:232:PHE:CE1	0.40	2.74	18	1
1:A:171:CYS:O	1:A:171:CYS:SG	0.40	2.78	7	1
1:A:217:ASN:OD1	1:A:217:ASN:C	0.40	2.64	8	2
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 [i](#)

6.3.1 Protein backbone [i](#)

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%)	0	5
All	All	1680/1740 (97%)	1080 (64%)	377 (22%)	223 (13%)	0	5

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	162	ASP	20
1	A	188	PRO	20
1	A	219	PRO	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	227	ASP	9
1	A	228	GLY	9
1	A	190	GLY	7
1	A	238	GLN	7
1	A	213	GLN	6
1	A	172	GLY	6
1	A	160	ASP	5
1	A	170	ILE	4
1	A	237	ASP	3
1	A	174	ALA	3
1	A	212	ALA	3
1	A	226	CYS	1

6.3.2 Protein sidechains [i](#)

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%)	49±2 (66±3%)	25±2 (34±3%)	1	11
All	All	1480/1540 (96%)	983 (66%)	497 (34%)	1	11

All 57 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	173	THR	19
1	A	198	LYS	19
1	A	171	CYS	17
1	A	210	MET	17
1	A	237	ASP	16
1	A	183	PHE	15
1	A	229	LYS	14
1	A	240	SER	14
1	A	166	LEU	13
1	A	216	VAL	13
1	A	177	LYS	13
1	A	196	LYS	12
1	A	233	LYS	12
1	A	230	LYS	12
1	A	187	CYS	11
1	A	226	CYS	11
1	A	239	LYS	11
1	A	194	ASN	11
1	A	207	SER	11
1	A	176	CYS	10
1	A	206	CYS	10
1	A	234	LEU	10
1	A	167	LYS	10
1	A	204	ASP	9
1	A	195	LEU	9
1	A	186	GLU	9
1	A	208	GLU	8
1	A	236	GLN	8
1	A	170	ILE	8
1	A	189	GLU	8
1	A	205	GLU	8
1	A	224	CYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	163	GLU	7
1	A	201	GLU	7
1	A	238	GLN	7
1	A	165	SER	6
1	A	213	GLN	6
1	A	164	CYS	6
1	A	242	GLU	5
1	A	197	SER	5
1	A	192	ARG	4
1	A	185	CYS	4
1	A	199	SER	4
1	A	209	ASN	4
1	A	223	THR	3
1	A	202	ASP	3
1	A	179	ILE	2
1	A	200	CYS	1
1	A	169	SER	1
1	A	175	VAL	1
1	A	162	ASP	1
1	A	184	GLU	1
1	A	214	LEU	1
1	A	225	TYR	1
1	A	227	ASP	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, 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