



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:52 AM GMT

PDB ID : 2P3F  
Title : Crystal structure of the factor Xa/NAP5 complex  
Authors : Rios-Steiner, J.L.; Murakami, M.T.; Tulinsky, A.; Arni, R.K.  
Deposited on : 2007-03-08  
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

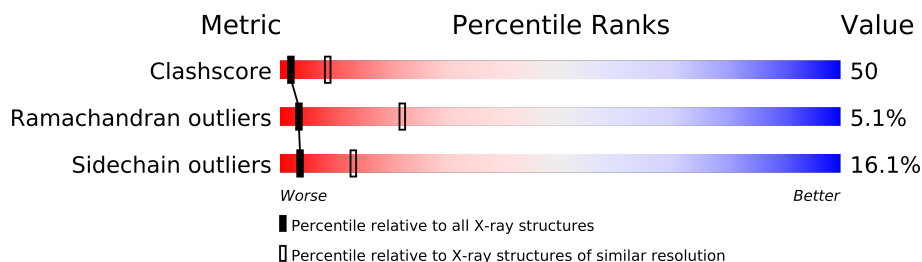
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	235	
2	L	54	
3	N	78	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2876 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	235	Total	C	N	O	S	0	0	0
			1864	1172	327	351	14			

- Molecule 2 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	51	Total	C	N	O	S	0	0	0
			376	225	64	80	7			

- Molecule 3 is a protein called Anti-coagulant protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	74	Total	C	N	O	S	0	0	0
			583	352	98	123	10			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

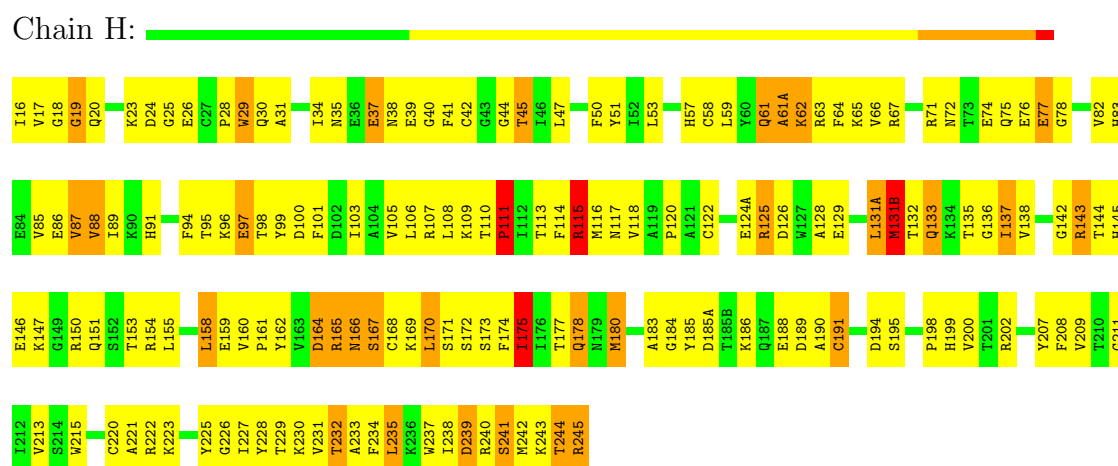
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	33	Total	O	0	0
			33	33		
5	L	9	Total	O	0	0
			9	9		
5	N	10	Total	O	0	0
			10	10		

### 3 Residue-property plots

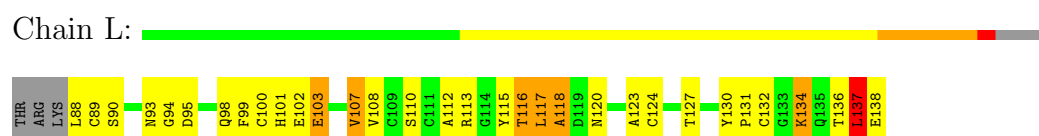
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

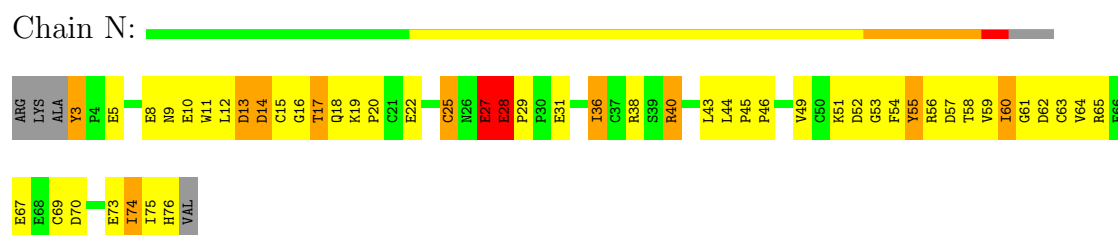
#### • Molecule 1: Coagulation factor X



#### • Molecule 2: Coagulation factor X



#### • Molecule 3: Anti-coagulant protein 5



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.17Å 137.17Å 167.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.180 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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 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	H	1.16	2/1902 (0.1%)	1.18	8/2560 (0.3%)
2	L	1.05	0/382	1.27	1/516 (0.2%)
3	N	1.07	1/596 (0.2%)	1.28	6/808 (0.7%)
All	All	1.13	3/2880 (0.1%)	1.22	15/3884 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	225	TYR	CD1-CE1	-6.26	1.29	1.39
1	H	225	TYR	CD2-CE2	-5.39	1.31	1.39
3	N	22	GLU	CB-CG	-5.17	1.42	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	115	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	L	137	LEU	N-CA-C	-7.39	91.05	111.00
1	H	199	HIS	N-CA-C	-6.32	93.93	111.00
3	N	70	ASP	N-CA-C	6.12	127.51	111.00
1	H	191	CYS	CA-CB-SG	6.08	124.94	114.00
1	H	165	ARG	NE-CZ-NH2	-6.04	117.28	120.30
3	N	60	ILE	N-CA-C	-5.98	94.85	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	133	GLN	N-CA-C	-5.71	95.57	111.00
3	N	69	CYS	CA-CB-SG	5.67	124.20	114.00
1	H	19	GLY	N-CA-C	-5.51	99.33	113.10
3	N	13	ASP	CB-CG-OD1	5.26	123.03	118.30
1	H	175	ILE	CB-CA-C	-5.26	101.09	111.60
3	N	59	VAL	CB-CA-C	-5.24	101.45	111.40
1	H	226	GLY	N-CA-C	-5.04	100.49	113.10
3	N	43	LEU	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	130	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1864	0	1821	208	0
2	L	376	0	336	30	0
3	N	583	0	512	53	0
4	H	1	0	0	0	0
5	H	33	0	0	2	0
5	L	9	0	0	1	0
5	N	10	0	0	0	0
All	All	2876	0	2669	277	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 50.

All (277) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:45:THR:HG23	1:H:198:PRO:HB3	1.40	1.00
1:H:98:THR:HG21	1:H:175:ILE:HD11	1.40	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:215:TRP:CD1	1:H:227:ILE:HD11	2.04	0.93
2:L:117:LEU:HD23	2:L:123:ALA:O	1.69	0.92
1:H:50:PHE:CZ	1:H:111:PRO:HB3	2.03	0.92
1:H:227:ILE:C	1:H:227:ILE:HD12	1.92	0.89
1:H:98:THR:CG2	1:H:175:ILE:HD11	2.05	0.87
3:N:64:VAL:HG23	3:N:65:ARG:O	1.76	0.86
1:H:215:TRP:CE2	1:H:227:ILE:HG12	2.11	0.85
1:H:215:TRP:NE1	1:H:227:ILE:HD11	1.91	0.84
1:H:143:ARG:HA	1:H:150:ARG:O	1.77	0.82
1:H:41:PHE:O	1:H:42:CYS:SG	2.37	0.82
1:H:86:GLU:HG2	1:H:87:VAL:HG12	1.61	0.81
1:H:230:LYS:HG2	1:H:232:THR:HG23	1.63	0.80
1:H:50:PHE:CE1	1:H:111:PRO:HB3	2.18	0.78
1:H:170:LEU:HD12	1:H:171:SER:N	1.97	0.78
1:H:86:GLU:C	1:H:87:VAL:HG12	2.05	0.77
1:H:180:MET:CE	1:H:215:TRP:HE1	1.98	0.76
1:H:35:ASN:ND2	1:H:39:GLU:HB2	2.03	0.74
1:H:45:THR:CG2	1:H:198:PRO:HB3	2.15	0.74
1:H:23:LYS:HB2	1:H:26:GLU:HG3	1.68	0.73
1:H:195:SER:HA	1:H:213:VAL:HG12	1.72	0.72
1:H:128:ALA:HA	1:H:131(A):LEU:HB2	1.72	0.72
3:N:3:TYR:CD2	3:N:12:LEU:HD21	2.24	0.71
1:H:113:THR:O	1:H:115:ARG:HG2	1.91	0.71
1:H:72:ASN:HD21	1:H:74:GLU:HG2	1.56	0.71
1:H:238:ILE:O	1:H:242:MET:HG3	1.91	0.71
3:N:73:GLU:O	3:N:74:ILE:HD13	1.90	0.71
1:H:153:THR:HG23	1:H:154:ARG:HG2	1.72	0.70
1:H:165:ARG:HG2	1:H:169:LYS:HE2	1.73	0.70
3:N:13:ASP:OD2	3:N:18:GLN:HB2	1.92	0.70
3:N:17:THR:HB	3:N:36:ILE:HD13	1.74	0.70
2:L:136:THR:O	2:L:137:LEU:HB2	1.93	0.69
1:H:23:LYS:C	1:H:71:ARG:HH12	1.95	0.68
1:H:164:ASP:CG	1:H:167:SER:HB2	2.14	0.68
1:H:51:TYR:CE1	1:H:107:ARG:HB2	2.29	0.68
1:H:209:VAL:HG12	1:H:231:VAL:HG11	1.76	0.68
1:H:147:LYS:HD3	3:N:11:TRP:CE2	2.28	0.68
1:H:220:CYS:O	1:H:221:ALA:HB3	1.92	0.67
1:H:150:ARG:HH21	3:N:12:LEU:HD23	1.59	0.67
2:L:101:HIS:O	2:L:107:VAL:HA	1.94	0.67
1:H:113:THR:O	1:H:115:ARG:NH1	2.28	0.67
1:H:72:ASN:HD21	1:H:74:GLU:H	1.41	0.66
1:H:89:ILE:HD12	1:H:89:ILE:N	2.10	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:166:ASN:HA	1:H:169:LYS:HE3	1.77	0.66
1:H:25:GLY:HA2	2:L:136:THR:OG1	1.96	0.66
1:H:72:ASN:ND2	1:H:74:GLU:H	1.92	0.66
1:H:94:PHE:HA	1:H:100:ASP:O	1.95	0.66
1:H:35:ASN:HD21	1:H:39:GLU:HB2	1.61	0.65
3:N:44:LEU:HB3	3:N:45:PRO:HD2	1.78	0.65
1:H:180:MET:HE2	1:H:215:TRP:HE1	1.62	0.64
1:H:135:THR:HG22	1:H:161:PRO:HA	1.79	0.64
1:H:62:LYS:HD2	1:H:62:LYS:H	1.63	0.64
1:H:86:GLU:HB2	1:H:109:LYS:HG2	1.80	0.64
1:H:72:ASN:HD21	1:H:74:GLU:N	1.96	0.64
3:N:13:ASP:O	3:N:46:PRO:HA	1.97	0.64
1:H:184:GLY:HA3	5:H:256:HOH:O	1.96	0.63
3:N:55:TYR:N	3:N:55:TYR:CD1	2.65	0.63
1:H:240:ARG:HA	1:H:243:LYS:HE2	1.80	0.63
1:H:215:TRP:NE1	1:H:227:ILE:CD1	2.60	0.63
1:H:174:PHE:CD1	3:N:38:ARG:CZ	2.81	0.63
3:N:12:LEU:HD11	3:N:46:PRO:HB2	1.81	0.63
1:H:230:LYS:CG	1:H:232:THR:HG23	2.29	0.63
1:H:24:ASP:HA	1:H:71:ARG:NH1	2.13	0.63
1:H:85:VAL:HG11	1:H:88:VAL:HG12	1.80	0.62
1:H:72:ASN:ND2	1:H:74:GLU:N	2.47	0.62
1:H:170:LEU:HD12	1:H:170:LEU:C	2.20	0.62
3:N:8:GLU:O	3:N:9:ASN:HB2	2.00	0.62
1:H:115:ARG:HG2	1:H:115:ARG:HH11	1.64	0.62
1:H:103:ILE:HD13	1:H:234:PHE:CB	2.30	0.62
1:H:95:THR:O	1:H:98:THR:N	2.30	0.61
1:H:165:ARG:O	1:H:168:CYS:HB3	2.00	0.61
2:L:136:THR:O	2:L:137:LEU:CB	2.49	0.61
3:N:60:ILE:O	3:N:62:ASP:N	2.33	0.61
3:N:3:TYR:CE2	3:N:12:LEU:HD21	2.35	0.61
2:L:113:ARG:HD3	5:L:147:HOH:O	2.00	0.60
3:N:9:ASN:ND2	3:N:54:PHE:CE2	2.70	0.60
2:L:116:THR:HB	2:L:127:THR:CG2	2.32	0.60
2:L:99:PHE:HB3	2:L:101:HIS:CE1	2.37	0.60
1:H:96:LYS:HB3	1:H:97:GLU:OE1	2.02	0.59
3:N:25:CYS:SG	3:N:57:ASP:HA	2.43	0.59
2:L:115:TYR:OH	2:L:134:LYS:HE2	2.03	0.59
2:L:116:THR:HB	2:L:127:THR:HG21	1.83	0.59
1:H:202:ARG:HB2	1:H:207:TYR:CE1	2.38	0.59
3:N:14:ASP:HA	3:N:46:PRO:HB3	1.84	0.58
1:H:107:ARG:NH1	1:H:108:LEU:O	2.36	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:151:GLN:HG2	3:N:14:ASP:OD2	2.02	0.58
1:H:232:THR:HA	1:H:235:LEU:HD22	1.84	0.58
1:H:94:PHE:CE1	1:H:99:TYR:HA	2.39	0.58
1:H:243:LYS:O	1:H:245:ARG:N	2.37	0.58
2:L:98:GLN:OE1	2:L:112:ALA:N	2.34	0.58
1:H:34:ILE:HD13	1:H:67:ARG:NH1	2.19	0.58
1:H:59:LEU:CD2	1:H:64:PHE:CZ	2.87	0.57
1:H:17:VAL:O	1:H:188:GLU:HA	2.04	0.57
3:N:55:TYR:H	3:N:55:TYR:HD1	1.52	0.57
1:H:180:MET:HE1	1:H:215:TRP:HE1	1.69	0.57
3:N:25:CYS:O	3:N:27:GLU:N	2.37	0.57
1:H:19:GLY:C	1:H:20:GLN:HG2	2.24	0.57
1:H:91:HIS:HB2	1:H:103:ILE:HG23	1.86	0.57
1:H:28:PRO:HG2	1:H:29:TRP:CE3	2.40	0.56
1:H:98:THR:CB	1:H:175:ILE:HD11	2.35	0.56
2:L:89:CYS:N	2:L:102:GLU:OE2	2.31	0.56
2:L:88:LEU:HA	2:L:102:GLU:OE2	2.05	0.56
1:H:59:LEU:HD21	1:H:64:PHE:CZ	2.40	0.56
1:H:83:HIS:HB3	1:H:108:LEU:HD22	1.86	0.56
1:H:124(A):GLU:OE1	1:H:126:ASP:HB2	2.06	0.56
1:H:145:HIS:CE1	1:H:147:LYS:H	2.24	0.55
1:H:215:TRP:CE2	1:H:227:ILE:CG1	2.87	0.55
1:H:232:THR:O	1:H:232:THR:OG1	2.24	0.54
1:H:231:VAL:C	1:H:233:ALA:H	2.10	0.54
1:H:165:ARG:HG2	1:H:169:LYS:CE	2.37	0.54
1:H:59:LEU:HD22	1:H:64:PHE:CE1	2.43	0.54
1:H:41:PHE:HE1	1:H:58:CYS:O	1.91	0.54
1:H:164:ASP:OD2	1:H:167:SER:HB2	2.06	0.54
2:L:115:TYR:CZ	2:L:131:PRO:HB2	2.42	0.54
1:H:53:LEU:HD21	1:H:231:VAL:HG21	1.88	0.54
2:L:89:CYS:SG	2:L:101:HIS:N	2.81	0.54
1:H:86:GLU:HB2	1:H:109:LYS:HA	1.90	0.54
1:H:131(B):MET:SD	1:H:232:THR:HG21	2.47	0.54
1:H:23:LYS:O	1:H:26:GLU:HB2	2.07	0.54
3:N:27:GLU:O	3:N:28:GLU:HB2	2.08	0.54
3:N:55:TYR:N	3:N:55:TYR:HD1	2.06	0.53
1:H:91:HIS:HA	1:H:237:TRP:CZ2	2.43	0.53
2:L:120:ASN:C	2:L:120:ASN:OD1	2.46	0.53
1:H:177:THR:O	1:H:180:MET:HG2	2.08	0.53
3:N:10:GLU:OE2	3:N:56:ARG:NH2	2.39	0.53
1:H:160:VAL:HG23	1:H:160:VAL:O	2.07	0.53
2:L:115:TYR:CE1	2:L:134:LYS:HE2	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:17:THR:HB	3:N:36:ILE:CD1	2.38	0.53
3:N:56:ARG:NH2	3:N:63:CYS:SG	2.82	0.53
1:H:241:SER:O	1:H:244:THR:HG23	2.09	0.53
1:H:183:ALA:HB3	1:H:228:TYR:CE2	2.43	0.53
2:L:103:GLU:HB2	2:L:108:VAL:HG11	1.90	0.53
1:H:94:PHE:CG	1:H:95:THR:N	2.77	0.53
1:H:72:ASN:HD22	1:H:75:GLN:H	1.56	0.53
1:H:86:GLU:CG	1:H:87:VAL:HG12	2.35	0.52
1:H:215:TRP:CZ2	1:H:227:ILE:HG12	2.43	0.52
1:H:147:LYS:HE2	3:N:52:ASP:OD1	2.08	0.52
1:H:178:GLN:O	1:H:230:LYS:NZ	2.27	0.52
1:H:72:ASN:ND2	1:H:75:GLN:N	2.57	0.52
1:H:105:VAL:HG12	1:H:106:LEU:N	2.23	0.52
3:N:73:GLU:HG3	3:N:74:ILE:N	2.25	0.52
1:H:94:PHE:HA	1:H:101:PHE:HB2	1.92	0.52
1:H:239:ASP:O	1:H:240:ARG:C	2.49	0.52
2:L:99:PHE:HB3	2:L:101:HIS:HE1	1.75	0.52
1:H:61:GLN:O	1:H:61(A):ALA:HB3	2.09	0.52
1:H:150:ARG:NH1	5:H:257:HOH:O	2.43	0.51
1:H:114:PHE:HA	1:H:118:VAL:O	2.10	0.51
1:H:207:TYR:CD2	1:H:207:TYR:N	2.78	0.51
1:H:72:ASN:ND2	1:H:75:GLN:H	2.10	0.51
3:N:51:LYS:HB2	3:N:54:PHE:CD1	2.46	0.51
1:H:170:LEU:CD1	1:H:170:LEU:C	2.80	0.50
1:H:116:MET:O	1:H:117:ASN:HB2	2.11	0.50
1:H:115:ARG:HG3	1:H:118:VAL:HB	1.92	0.50
3:N:9:ASN:O	3:N:51:LYS:HG3	2.12	0.50
1:H:95:THR:O	1:H:99:TYR:N	2.42	0.50
1:H:50:PHE:CZ	1:H:111:PRO:CB	2.89	0.50
1:H:103:ILE:HD13	1:H:234:PHE:HB2	1.94	0.50
2:L:100:CYS:O	2:L:101:HIS:CD2	2.65	0.50
1:H:50:PHE:CE2	1:H:111:PRO:HB3	2.46	0.49
1:H:166:ASN:HA	1:H:169:LYS:CE	2.41	0.49
1:H:35:ASN:OD1	1:H:38:ASN:N	2.46	0.49
1:H:173:SER:C	1:H:174:PHE:CD2	2.86	0.49
1:H:143:ARG:HD3	1:H:145:HIS:O	2.13	0.49
1:H:95:THR:HG22	1:H:98:THR:H	1.77	0.49
1:H:83:HIS:CB	1:H:108:LEU:HD22	2.43	0.49
1:H:24:ASP:CA	1:H:71:ARG:NH1	2.76	0.49
1:H:72:ASN:C	1:H:72:ASN:ND2	2.65	0.49
1:H:136:GLY:C	1:H:137:ILE:HG12	2.32	0.49
1:H:94:PHE:HE1	1:H:99:TYR:HA	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:13:ASP:O	3:N:15:CYS:N	2.46	0.49
1:H:158:LEU:HD22	1:H:160:VAL:CG1	2.42	0.49
1:H:88:VAL:C	1:H:89:ILE:HD12	2.33	0.48
1:H:165:ARG:O	1:H:168:CYS:N	2.47	0.48
1:H:145:HIS:O	1:H:146:GLU:C	2.48	0.48
1:H:237:TRP:O	1:H:241:SER:HB3	2.14	0.48
3:N:75:ILE:HG22	3:N:76:HIS:N	2.27	0.48
1:H:117:ASN:C	1:H:118:VAL:CG2	2.81	0.48
1:H:105:VAL:HG23	1:H:237:TRP:HZ3	1.79	0.48
1:H:131(A):LEU:HD12	1:H:131(A):LEU:HA	1.63	0.48
3:N:13:ASP:C	3:N:15:CYS:H	2.16	0.48
3:N:10:GLU:HG2	3:N:63:CYS:SG	2.54	0.48
1:H:174:PHE:CE1	3:N:38:ARG:CZ	2.96	0.47
2:L:117:LEU:O	2:L:118:ALA:C	2.52	0.47
1:H:143:ARG:HA	1:H:151:GLN:HA	1.96	0.47
1:H:131(A):LEU:O	1:H:133:GLN:HB2	2.14	0.47
1:H:142:GLY:HA3	1:H:194:ASP:OD2	2.14	0.47
1:H:220:CYS:O	1:H:221:ALA:CB	2.58	0.47
2:L:93:ASN:O	2:L:100:CYS:HB2	2.13	0.47
3:N:40:ARG:HG2	3:N:40:ARG:HH11	1.80	0.47
1:H:151:GLN:NE2	3:N:15:CYS:SG	2.87	0.47
1:H:165:ARG:HH22	1:H:177:THR:C	2.18	0.47
1:H:16:ILE:O	1:H:144:THR:HA	2.15	0.47
1:H:122:CYS:SG	2:L:132:CYS:O	2.72	0.47
1:H:75:GLN:HB3	1:H:77:GLU:OE2	2.15	0.47
1:H:125:ARG:NH1	1:H:129:GLU:OE1	2.48	0.47
3:N:36:ILE:HD13	3:N:36:ILE:O	2.15	0.46
1:H:173:SER:O	1:H:174:PHE:CD2	2.68	0.46
3:N:53:GLY:O	3:N:54:PHE:CG	2.68	0.46
3:N:16:GLY:O	3:N:18:GLN:N	2.48	0.46
1:H:72:ASN:HD22	1:H:75:GLN:N	2.13	0.46
1:H:135:THR:HG22	1:H:161:PRO:CA	2.46	0.46
1:H:227:ILE:O	1:H:227:ILE:HD12	2.15	0.46
1:H:209:VAL:O	1:H:209:VAL:HG12	2.15	0.46
1:H:116:MET:CE	2:L:137:LEU:HA	2.46	0.46
1:H:185(A):ASP:OD1	1:H:185(A):ASP:C	2.53	0.46
2:L:115:TYR:HB3	2:L:124:CYS:HB3	1.97	0.45
1:H:37:GLU:O	1:H:38:ASN:HB2	2.15	0.45
1:H:116:MET:HE1	2:L:137:LEU:CA	2.47	0.45
1:H:158:LEU:HD23	1:H:159:GLU:N	2.32	0.45
1:H:103:ILE:HG21	1:H:234:PHE:CD2	2.51	0.45
1:H:158:LEU:HD22	1:H:160:VAL:HG13	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:72:ASN:ND2	1:H:74:GLU:HG2	2.29	0.45
1:H:76:GLU:O	1:H:77:GLU:HB3	2.17	0.45
1:H:65:LYS:HB3	1:H:82:VAL:HG12	1.99	0.45
1:H:35:ASN:OD1	1:H:39:GLU:N	2.26	0.45
1:H:131(A):LEU:C	1:H:132:THR:H	2.19	0.45
1:H:175:ILE:H	1:H:175:ILE:HG12	1.57	0.44
1:H:96:LYS:HB3	1:H:96:LYS:HE2	1.82	0.44
1:H:83:HIS:CB	1:H:108:LEU:HD13	2.48	0.44
1:H:59:LEU:CD2	1:H:64:PHE:CE1	3.00	0.44
3:N:31:GLU:OE1	3:N:31:GLU:HA	2.16	0.44
1:H:96:LYS:HE2	1:H:97:GLU:OE1	2.17	0.44
1:H:34:ILE:HG22	1:H:40:GLY:HA2	2.00	0.44
1:H:117:ASN:C	1:H:118:VAL:HG23	2.38	0.44
1:H:97:GLU:CD	1:H:97:GLU:H	2.21	0.44
1:H:191:CYS:O	1:H:194:ASP:HB2	2.17	0.44
1:H:30:GLN:HG2	1:H:155:LEU:CD1	2.48	0.44
1:H:124(A):GLU:O	1:H:125:ARG:C	2.55	0.44
1:H:24:ASP:N	1:H:71:ARG:NH1	2.65	0.44
3:N:19:LYS:N	3:N:20:PRO:HD2	2.33	0.44
1:H:94:PHE:CD1	1:H:95:THR:N	2.84	0.43
1:H:66:VAL:O	1:H:83:HIS:N	2.39	0.43
3:N:16:GLY:C	3:N:18:GLN:H	2.20	0.43
3:N:19:LYS:O	3:N:20:PRO:C	2.54	0.43
2:L:117:LEU:O	2:L:118:ALA:O	2.36	0.43
1:H:231:VAL:O	1:H:231:VAL:HG13	2.18	0.43
1:H:89:ILE:CD1	1:H:89:ILE:N	2.77	0.43
1:H:113:THR:HG22	1:H:113:THR:O	2.19	0.43
3:N:55:TYR:O	3:N:63:CYS:HA	2.18	0.43
1:H:174:PHE:CE1	3:N:38:ARG:NH2	2.87	0.43
1:H:189:ASP:OD2	1:H:190:ALA:N	2.51	0.43
1:H:173:SER:O	1:H:174:PHE:CG	2.72	0.43
1:H:24:ASP:N	1:H:71:ARG:HH12	2.17	0.42
3:N:28:GLU:N	3:N:29:PRO:HD3	2.34	0.42
2:L:115:TYR:CZ	2:L:134:LYS:HE2	2.54	0.42
2:L:103:GLU:HB2	2:L:108:VAL:CG1	2.49	0.42
1:H:131(B):MET:HE3	1:H:162:TYR:CE1	2.54	0.42
3:N:9:ASN:C	3:N:51:LYS:HG3	2.40	0.42
1:H:88:VAL:CG2	1:H:88:VAL:O	2.65	0.42
1:H:31:ALA:N	1:H:44:GLY:O	2.52	0.42
1:H:91:HIS:HA	1:H:237:TRP:HZ2	1.82	0.42
1:H:138:VAL:HG12	1:H:158:LEU:HB3	2.02	0.42
1:H:164:ASP:OD1	1:H:167:SER:HB2	2.19	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:53:GLY:O	3:N:54:PHE:CD1	2.73	0.41
1:H:125:ARG:O	1:H:128:ALA:HB3	2.20	0.41
2:L:89:CYS:O	2:L:94:GLY:N	2.53	0.41
1:H:122:CYS:O	1:H:208:PHE:HA	2.20	0.41
1:H:50:PHE:CG	1:H:107:ARG:NH2	2.88	0.41
3:N:40:ARG:NH1	3:N:40:ARG:HG2	2.36	0.41
1:H:185:TYR:CG	1:H:186:LYS:HB3	2.56	0.41
1:H:50:PHE:HD2	1:H:108:LEU:O	2.04	0.41
1:H:150:ARG:HH21	3:N:12:LEU:CD2	2.29	0.41
1:H:24:ASP:OD1	1:H:117:ASN:ND2	2.53	0.41
1:H:75:GLN:HG2	1:H:76:GLU:O	2.21	0.41
1:H:165:ARG:CG	1:H:169:LYS:HE2	2.47	0.41
1:H:41:PHE:CE1	1:H:58:CYS:O	2.72	0.41
1:H:195:SER:HA	1:H:213:VAL:O	2.20	0.41
1:H:17:VAL:HG13	1:H:144:THR:O	2.21	0.40
1:H:211:GLY:HA2	1:H:229:THR:O	2.20	0.40
1:H:63:ARG:HB2	1:H:63:ARG:CZ	2.51	0.40
1:H:200:VAL:HG23	1:H:200:VAL:O	2.20	0.40
1:H:174:PHE:CD1	3:N:38:ARG:NH2	2.89	0.40
1:H:222:ARG:NH2	1:H:222:ARG:HG3	2.36	0.40
1:H:116:MET:O	1:H:117:ASN:CB	2.70	0.40
1:H:47:LEU:HD11	1:H:53:LEU:HB2	2.03	0.40
3:N:56:ARG:HA	3:N:62:ASP:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution. 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	H	233/235 (99%)	194 (83%)	32 (14%)	7 (3%)	7	37
2	L	49/54 (91%)	39 (80%)	6 (12%)	4 (8%)	1	10
3	N	72/78 (92%)	55 (76%)	10 (14%)	7 (10%)	1	6
All	All	354/367 (96%)	288 (81%)	48 (14%)	18 (5%)	3	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	244	THR
2	L	137	LEU
3	N	27	GLU
1	H	77	GLU
1	H	78	GLY
2	L	90	SER
3	N	14	ASP
3	N	17	THR
3	N	25	CYS
3	N	67	GLU
1	H	131(B)	MET
2	L	95	ASP
3	N	61	GLY
1	H	61(A)	ALA
2	L	118	ALA
1	H	18	GLY
1	H	111	PRO
3	N	28	GLU

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution. 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	H	200/200 (100%)	167 (84%)	33 (16%)	3	12
2	L	43/46 (94%)	36 (84%)	7 (16%)	3	12
3	N	67/70 (96%)	57 (85%)	10 (15%)	4	17
All	All	310/316 (98%)	260 (84%)	50 (16%)	3	13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	29	TRP
1	H	37	GLU
1	H	45	THR
1	H	57	HIS
1	H	61	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	62	LYS
1	H	87	VAL
1	H	88	VAL
1	H	97	GLU
1	H	110	THR
1	H	111	PRO
1	H	115	ARG
1	H	120	PRO
1	H	125	ARG
1	H	131(A)	LEU
1	H	131(B)	MET
1	H	137	ILE
1	H	143	ARG
1	H	158	LEU
1	H	164	ASP
1	H	166	ASN
1	H	167	SER
1	H	170	LEU
1	H	172	SER
1	H	175	ILE
1	H	178	GLN
1	H	180	MET
1	H	223	LYS
1	H	232	THR
1	H	235	LEU
1	H	239	ASP
1	H	241	SER
1	H	245	ARG
2	L	103	GLU
2	L	107	VAL
2	L	110	SER
2	L	116	THR
2	L	117	LEU
2	L	134	LYS
2	L	138	GLU
3	N	3	TYR
3	N	5	GLU
3	N	27	GLU
3	N	28	GLU
3	N	36	ILE
3	N	40	ARG
3	N	49	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	N	55	TYR
3	N	58	THR
3	N	74	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	30	GLN
1	H	72	ASN
1	H	75	GLN
1	H	117	ASN
1	H	178	GLN
2	L	101	HIS
3	N	71	GLN
3	N	72	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.