



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:54 AM GMT

PDB ID : 1HCG
Title : STRUCTURE OF HUMAN DES(1-45) FACTOR XA AT 2.2 ANGSTROMS
RESOLUTION
Authors : Tulinsky, A.; Padmanabhan, K.
Deposited on : 1993-05-05
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

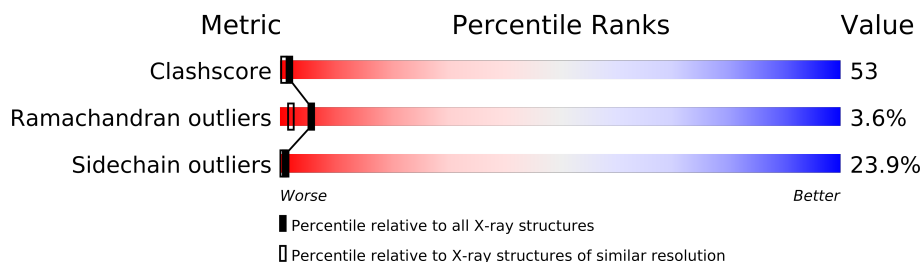
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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 ≥ 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	A	241	
2	B	51	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2449 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 BLOOD COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1863	1176	325	348	14			

- Molecule 2 is a protein called BLOOD COAGULATION FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	51	Total	C	N	O	S	0	0	0
			379	225	67	80	7			

- Molecule 3 is water.

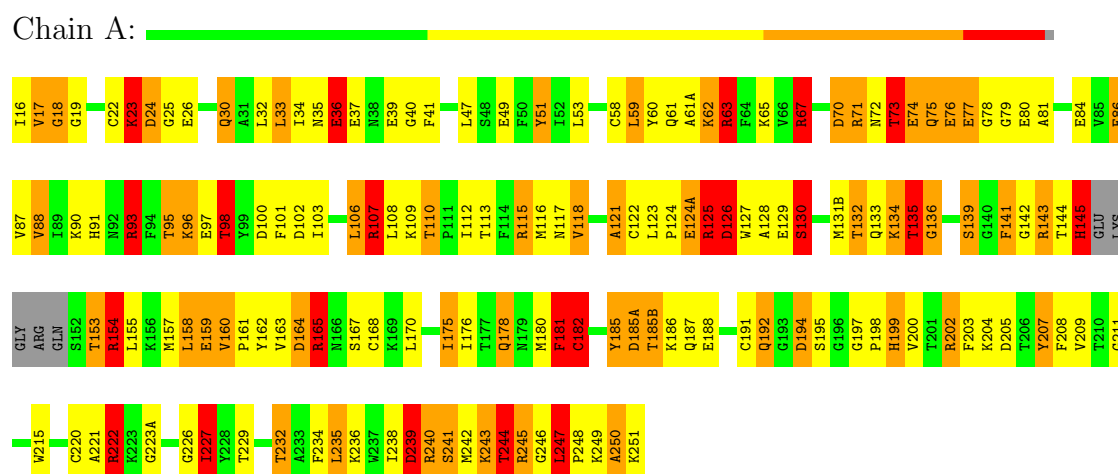
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	29	Total	O	0	0
			29	29		

3 Residue-property plots

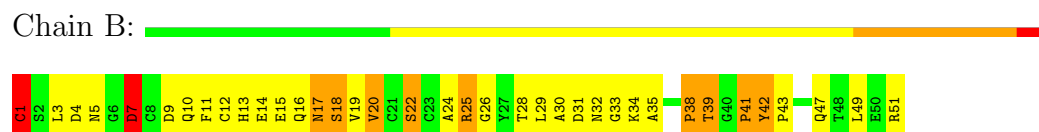
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BLOOD COAGULATION FACTOR XA



• Molecule 2: BLOOD COAGULATION FACTOR XA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.66Å 93.66Å 119.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.168 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2449	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	A	1.19	2/1901 (0.1%)	2.61	96/2560 (3.8%)
2	B	1.14	0/385	2.52	14/519 (2.7%)
All	All	1.18	2/2286 (0.1%)	2.60	110/3079 (3.6%)

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
1	A	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLY	N-CA	5.53	1.54	1.46
1	A	18	GLY	N-CA	-5.21	1.38	1.46

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ARG	NE-CZ-NH2	33.78	137.19	120.30
2	B	51	ARG	NE-CZ-NH1	-26.30	107.15	120.30
1	A	165	ARG	NE-CZ-NH2	-25.42	107.59	120.30
1	A	222	ARG	NE-CZ-NH1	-23.96	108.32	120.30
1	A	71	ARG	NE-CZ-NH1	22.05	131.32	120.30
1	A	107	ARG	NE-CZ-NH2	-19.07	110.76	120.30
1	A	115	ARG	NE-CZ-NH1	18.05	129.33	120.30
1	A	202	ARG	NE-CZ-NH1	16.24	128.42	120.30
1	A	239	ASP	CB-CG-OD1	-14.78	105.00	118.30
1	A	115	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	A	71	ARG	CD-NE-CZ	13.86	143.00	123.60
1	A	165	ARG	NE-CZ-NH1	13.67	127.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	ARG	NE-CZ-NH2	-13.13	113.74	120.30
2	B	51	ARG	CD-NE-CZ	-12.35	106.31	123.60
1	A	143	ARG	NE-CZ-NH2	12.10	126.35	120.30
1	A	247	LEU	CB-CA-C	11.84	132.69	110.20
1	A	93	ARG	NE-CZ-NH1	10.85	125.72	120.30
2	B	25	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	107	ARG	NH1-CZ-NH2	10.17	130.59	119.40
1	A	67	ARG	NE-CZ-NH2	-10.15	115.23	120.30
2	B	7	ASP	CB-CG-OD2	-9.85	109.44	118.30
1	A	194	ASP	CB-CG-OD1	-9.77	109.51	118.30
1	A	202	ARG	CD-NE-CZ	9.76	137.26	123.60
1	A	71	ARG	NE-CZ-NH2	-9.71	115.45	120.30
2	B	51	ARG	NE-CZ-NH2	9.58	125.09	120.30
1	A	24	ASP	CB-CG-OD1	9.22	126.60	118.30
1	A	98	THR	N-CA-CB	-8.94	93.32	110.30
1	A	125	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	239	ASP	CA-CB-CG	-8.62	94.44	113.40
2	B	7	ASP	CA-CB-CG	-8.46	94.79	113.40
1	A	22	CYS	O-C-N	8.30	135.99	122.70
1	A	180	MET	CG-SD-CE	8.25	113.40	100.20
1	A	185	TYR	CB-CG-CD2	-8.21	116.07	121.00
1	A	239	ASP	OD1-CG-OD2	8.20	138.88	123.30
1	A	245	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	125	ARG	CD-NE-CZ	8.03	134.85	123.60
1	A	107	ARG	CG-CD-NE	-7.90	95.22	111.80
1	A	154	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	250	ALA	N-CA-CB	-7.54	99.54	110.10
1	A	63	ARG	NE-CZ-NH2	7.52	124.06	120.30
2	B	51	ARG	NH1-CZ-NH2	7.38	127.52	119.40
1	A	245	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	139	SER	N-CA-CB	7.20	121.29	110.50
1	A	107	ARG	N-CA-CB	7.19	123.54	110.60
1	A	185	TYR	CB-CG-CD1	7.14	125.29	121.00
1	A	181	PHE	O-C-N	-7.12	111.31	122.70
1	A	141	PHE	CA-C-N	7.03	130.26	116.20
1	A	202	ARG	NH1-CZ-NH2	-6.92	111.79	119.40
1	A	102	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	141	PHE	C-N-CA	-6.89	107.84	122.30
1	A	240	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	239	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	195	SER	C-N-CA	6.70	136.38	122.30
2	B	9	ASP	CB-CG-OD1	6.69	124.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	PHE	CA-C-O	-6.54	106.37	120.10
1	A	227	ILE	C-N-CA	6.45	137.81	121.70
1	A	181	PHE	N-CA-C	6.41	128.31	111.00
1	A	195	SER	CB-CA-C	6.36	122.19	110.10
1	A	244	THR	N-CA-CB	6.34	122.34	110.30
1	A	130	SER	N-CA-CB	-6.27	101.09	110.50
1	A	93	ARG	CD-NE-CZ	6.25	132.35	123.60
2	B	1	CYS	CB-CA-C	-6.25	97.90	110.40
1	A	132	THR	CA-CB-OG1	-6.21	95.96	109.00
1	A	135	THR	N-CA-CB	-6.09	98.73	110.30
1	A	107	ARG	O-C-N	6.00	132.31	122.70
1	A	175	ILE	CA-CB-CG2	6.00	122.90	110.90
1	A	185	TYR	CA-C-N	-6.00	104.00	117.20
2	B	22	SER	C-N-CA	5.99	136.68	121.70
1	A	98	THR	CA-CB-CG2	5.90	120.67	112.40
1	A	165	ARG	CG-CD-NE	-5.85	99.51	111.80
1	A	93	ARG	NH1-CZ-NH2	-5.84	112.98	119.40
1	A	157	MET	C-N-CA	5.83	136.28	121.70
1	A	141	PHE	CA-C-O	-5.80	107.92	120.10
1	A	185(A)	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	241	SER	O-C-N	5.76	131.92	122.70
1	A	181	PHE	CA-C-N	5.72	129.79	117.20
1	A	51	TYR	CZ-CE2-CD2	-5.65	114.71	119.80
1	A	145	HIS	CA-CB-CG	-5.65	103.99	113.60
1	A	71	ARG	NH1-CZ-NH2	-5.65	113.19	119.40
1	A	110	THR	CA-CB-CG2	-5.63	104.51	112.40
1	A	162	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	207	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	136	GLY	N-CA-C	-5.62	99.06	113.10
1	A	199	HIS	N-CA-C	-5.60	95.89	111.00
1	A	182	CYS	CB-CA-C	-5.55	99.29	110.40
1	A	165	ARG	CB-CG-CD	5.55	126.02	111.60
1	A	222	ARG	CD-NE-CZ	-5.53	115.85	123.60
1	A	244	THR	C-N-CA	-5.50	107.96	121.70
2	B	42	TYR	CZ-CE2-CD2	-5.46	114.88	119.80
1	A	185(B)	THR	CA-CB-OG1	-5.42	97.61	109.00
1	A	122	CYS	CA-CB-SG	5.40	123.71	114.00
1	A	239	ASP	N-CA-CB	-5.34	100.98	110.60
1	A	22	CYS	CA-C-O	-5.31	108.95	120.10
1	A	160	VAL	CA-CB-CG1	5.30	118.85	110.90
1	A	197	GLY	CA-C-O	5.30	130.14	120.60
1	A	67	ARG	CA-CB-CG	5.26	124.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	GLU	CA-CB-CG	5.25	124.94	113.40
1	A	159	GLU	CG-CD-OE1	-5.24	107.82	118.30
1	A	164	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	19	GLY	N-CA-C	-5.16	100.21	113.10
1	A	124(A)	GLU	CB-CA-C	-5.15	100.09	110.40
1	A	121	ALA	CA-C-N	5.14	128.50	117.20
2	B	9	ASP	CA-CB-CG	5.10	124.62	113.40
1	A	118	VAL	CA-CB-CG2	5.09	118.54	110.90
1	A	17	VAL	C-N-CA	5.08	132.97	122.30
1	A	243	LYS	CA-C-N	5.07	128.35	117.20
1	A	30	GLN	C-N-CA	5.06	134.35	121.70
1	A	23	LYS	CB-CA-C	-5.06	100.28	110.40
1	A	126	ASP	CB-CG-OD1	5.02	122.82	118.30
2	B	41	PRO	CA-C-O	-5.02	108.16	120.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	154	ARG	Sidechain
1	A	163	VAL	Mainchain
1	A	165	ARG	Sidechain
1	A	222	ARG	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	A	1863	0	1829	185	0
2	B	379	0	341	48	0
3	A	178	0	0	39	0
3	B	29	0	0	7	0
All	All	2449	0	2170	230	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 53.

All (230) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:39:THR:HG21	3:B:668:HOH:O	1.28	1.26
1:A:25:GLY:N	1:A:117:ASN:HD21	1.32	1.25
1:A:25:GLY:H	1:A:117:ASN:ND2	1.37	1.20
1:A:247:LEU:HD11	3:A:709:HOH:O	1.39	1.20
1:A:245:ARG:HB3	3:A:734:HOH:O	1.38	1.20
2:B:4:ASP:HB2	3:B:587:HOH:O	1.38	1.19
1:A:215:TRP:NE1	1:A:227:ILE:HD11	1.57	1.17
1:A:36:GLU:HG2	3:A:528:HOH:O	1.43	1.14
1:A:72:ASN:ND2	1:A:75:GLN:HB2	1.64	1.12
1:A:143:ARG:NE	1:A:192:GLN:HB2	1.67	1.08
2:B:16:GLN:HB3	3:B:691:HOH:O	1.53	1.07
1:A:143:ARG:HE	1:A:192:GLN:CB	1.70	1.03
1:A:215:TRP:HE1	1:A:227:ILE:HD11	1.15	1.02
1:A:34:ILE:HG21	1:A:67:ARG:NH1	1.75	1.01
1:A:25:GLY:HA2	1:A:117:ASN:HD22	1.27	1.00
1:A:143:ARG:HE	1:A:192:GLN:HB2	0.84	0.99
1:A:202:ARG:NH2	1:A:205:ASP:OD1	1.95	0.99
1:A:215:TRP:NE1	1:A:227:ILE:CD1	2.25	0.98
1:A:98:THR:HG21	3:A:511:HOH:O	1.64	0.98
1:A:25:GLY:N	1:A:117:ASN:ND2	1.99	0.95
1:A:73:THR:O	1:A:73:THR:CG2	2.15	0.94
1:A:72:ASN:HD22	1:A:75:GLN:HB2	1.19	0.94
1:A:250:ALA:HB2	3:A:750:HOH:O	1.69	0.93
1:A:16:ILE:HG12	1:A:194:ASP:OD2	1.68	0.93
1:A:86:GLU:OE2	1:A:245:ARG:NH1	2.03	0.92
1:A:72:ASN:HD22	1:A:75:GLN:CB	1.83	0.91
1:A:181:PHE:O	1:A:182:CYS:HB2	1.71	0.90
1:A:75:GLN:HB3	3:A:818:HOH:O	1.72	0.89
1:A:131(B):MET:CE	3:A:508:HOH:O	2.19	0.89
1:A:25:GLY:CA	1:A:117:ASN:ND2	2.35	0.88
1:A:25:GLY:HA2	1:A:117:ASN:ND2	1.90	0.85
1:A:34:ILE:HG21	1:A:67:ARG:HH11	1.36	0.85
1:A:125:ARG:NH2	1:A:129:GLU:OE2	2.10	0.85
1:A:72:ASN:HB3	3:A:818:HOH:O	1.77	0.84
1:A:215:TRP:CE2	1:A:227:ILE:HG12	2.12	0.83
1:A:204:LYS:O	1:A:205:ASP:HB2	1.76	0.83
1:A:71:ARG:HD3	3:A:647:HOH:O	1.79	0.83
2:B:1:CYS:SG	2:B:13:HIS:N	2.52	0.83
2:B:13:HIS:CE1	3:B:510:HOH:O	2.32	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:ARG:CZ	1:A:129:GLU:OE2	2.29	0.81
1:A:215:TRP:CD2	1:A:227:ILE:HG12	2.16	0.80
1:A:73:THR:O	1:A:73:THR:HG22	1.80	0.80
1:A:98:THR:CG2	1:A:100:ASP:HB2	2.12	0.79
2:B:1:CYS:H1	2:B:19:VAL:CG2	1.94	0.79
1:A:185(A):ASP:OD1	1:A:223(A):GLY:HA2	1.83	0.78
1:A:222:ARG:O	3:A:583:HOH:O	1.99	0.78
1:A:143:ARG:HG3	1:A:192:GLN:HB3	1.66	0.78
2:B:29:LEU:HD11	2:B:33:GLY:C	2.04	0.78
1:A:23:LYS:HG2	1:A:26:GLU:CD	2.04	0.78
1:A:75:GLN:HG3	3:A:648:HOH:O	1.84	0.77
1:A:232:THR:HA	1:A:235:LEU:HD22	1.67	0.77
1:A:131(B):MET:HE1	3:A:508:HOH:O	1.80	0.77
1:A:34:ILE:HD13	1:A:67:ARG:HD3	1.68	0.76
1:A:73:THR:N	1:A:153:THR:O	2.15	0.75
1:A:191:CYS:O	1:A:194:ASP:HB2	1.87	0.74
1:A:90:LYS:O	1:A:248:PRO:HA	1.87	0.74
1:A:125:ARG:O	1:A:129:GLU:HG2	1.89	0.73
1:A:35:ASN:OD1	1:A:39:GLU:HB2	1.87	0.72
1:A:17:VAL:HG22	1:A:145:HIS:HB2	1.71	0.72
2:B:14:GLU:OE1	2:B:14:GLU:HA	1.90	0.71
1:A:71:ARG:CD	3:A:647:HOH:O	2.36	0.71
1:A:79:GLY:CA	3:A:712:HOH:O	2.38	0.70
2:B:14:GLU:HA	2:B:18:SER:O	1.90	0.70
1:A:76:GLU:O	1:A:78:GLY:N	2.25	0.70
1:A:143:ARG:NE	1:A:192:GLN:CB	2.41	0.70
1:A:185:TYR:O	3:A:583:HOH:O	2.09	0.70
1:A:215:TRP:HE1	1:A:227:ILE:CD1	1.94	0.69
2:B:1:CYS:HB2	2:B:14:GLU:CD	2.13	0.69
1:A:186:LYS:O	3:A:741:HOH:O	2.10	0.69
2:B:29:LEU:HD12	2:B:35:ALA:O	1.92	0.68
1:A:73:THR:O	1:A:73:THR:HG23	1.94	0.68
1:A:30:GLN:HB2	3:A:740:HOH:O	1.92	0.68
1:A:81:ALA:CB	1:A:115:ARG:HH22	2.06	0.68
1:A:125:ARG:HH21	1:A:232:THR:HG23	1.59	0.67
1:A:81:ALA:HB3	1:A:115:ARG:HH22	1.58	0.67
1:A:76:GLU:C	1:A:78:GLY:H	1.96	0.67
1:A:79:GLY:HA2	3:A:712:HOH:O	1.92	0.67
1:A:25:GLY:CA	1:A:117:ASN:HD22	1.99	0.66
1:A:75:GLN:CB	3:A:818:HOH:O	2.36	0.66
1:A:182:CYS:HA	1:A:226:GLY:O	1.95	0.66
1:A:202:ARG:HG2	3:A:731:HOH:O	1.94	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:PHE:O	1:A:182:CYS:CB	2.35	0.66
1:A:73:THR:HB	1:A:153:THR:O	1.95	0.66
2:B:30:ALA:CB	2:B:35:ALA:HB3	2.26	0.66
1:A:241:SER:C	1:A:243:LYS:H	1.99	0.66
1:A:93:ARG:HG3	3:A:568:HOH:O	1.96	0.65
2:B:15:GLU:N	2:B:18:SER:O	2.30	0.64
1:A:84:GLU:N	3:A:677:HOH:O	2.31	0.64
1:A:98:THR:HG22	1:A:100:ASP:HB2	1.80	0.63
1:A:215:TRP:CE2	1:A:227:ILE:CG1	2.81	0.63
1:A:215:TRP:CE2	1:A:227:ILE:CD1	2.82	0.63
2:B:1:CYS:N	2:B:14:GLU:OE2	2.29	0.63
1:A:77:GLU:CB	3:A:762:HOH:O	2.47	0.62
2:B:29:LEU:HD11	2:B:33:GLY:O	2.00	0.61
1:A:81:ALA:HB2	1:A:115:ARG:NH2	2.16	0.61
1:A:124(A):GLU:OE1	2:B:13:HIS:NE2	2.33	0.61
1:A:215:TRP:CD1	1:A:227:ILE:HD11	2.33	0.60
1:A:220:CYS:SG	3:A:761:HOH:O	2.56	0.60
1:A:80:GLU:HB2	3:A:598:HOH:O	2.01	0.60
1:A:134:LYS:O	1:A:161:PRO:HA	2.02	0.60
2:B:30:ALA:HB3	2:B:35:ALA:HB3	1.82	0.60
1:A:73:THR:HG22	1:A:153:THR:HB	1.84	0.59
1:A:77:GLU:HB3	3:A:762:HOH:O	2.01	0.59
1:A:98:THR:HG22	1:A:100:ASP:H	1.67	0.59
1:A:250:ALA:CB	3:A:750:HOH:O	2.39	0.58
1:A:186:LYS:HE2	1:A:188:GLU:OE1	2.03	0.58
1:A:202:ARG:CZ	1:A:205:ASP:OD1	2.52	0.57
2:B:1:CYS:SG	2:B:12:CYS:C	2.82	0.57
1:A:16:ILE:O	1:A:144:THR:HA	2.04	0.57
2:B:12:CYS:SG	2:B:19:VAL:HG13	2.44	0.57
2:B:12:CYS:O	2:B:13:HIS:ND1	2.38	0.57
1:A:235:LEU:O	3:A:765:HOH:O	2.17	0.56
1:A:23:LYS:HG2	1:A:26:GLU:OE1	2.04	0.56
1:A:72:ASN:ND2	1:A:75:GLN:CB	2.48	0.56
1:A:238:ILE:HB	3:A:765:HOH:O	2.05	0.56
1:A:81:ALA:CB	1:A:115:ARG:NH2	2.69	0.56
1:A:34:ILE:CD1	1:A:67:ARG:HH11	2.20	0.55
1:A:109:LYS:C	1:A:110:THR:HG23	2.26	0.55
1:A:215:TRP:NE1	1:A:227:ILE:CG1	2.70	0.55
1:A:91:HIS:CE1	1:A:101:PHE:CD2	2.96	0.54
1:A:191:CYS:SG	1:A:192:GLN:N	2.75	0.54
1:A:17:VAL:CG2	1:A:145:HIS:HB2	2.36	0.54
1:A:32:LEU:HD21	3:A:810:HOH:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:14:GLU:OE1	2:B:14:GLU:CA	2.55	0.53
1:A:86:GLU:HG3	1:A:109:LYS:HG2	1.90	0.53
1:A:76:GLU:C	1:A:78:GLY:N	2.62	0.53
1:A:131(B):MET:HE3	3:A:508:HOH:O	2.00	0.53
2:B:41:PRO:HB2	2:B:42:TYR:CE2	2.44	0.53
1:A:34:ILE:HA	1:A:39:GLU:O	2.09	0.52
1:A:63:ARG:HB2	3:A:558:HOH:O	2.10	0.52
1:A:35:ASN:C	1:A:37:GLU:H	2.12	0.52
1:A:135:THR:HG23	1:A:159:GLU:HG3	1.92	0.52
2:B:34:LYS:HD3	3:B:782:HOH:O	2.09	0.52
1:A:51:TYR:HA	1:A:106:LEU:O	2.10	0.52
1:A:59:LEU:HD13	1:A:88:VAL:HG21	1.92	0.51
1:A:34:ILE:HD13	1:A:67:ARG:HH11	1.73	0.51
1:A:158:LEU:HD13	1:A:160:VAL:HG13	1.91	0.51
1:A:80:GLU:CB	3:A:598:HOH:O	2.56	0.51
2:B:11:PHE:HB2	2:B:22:SER:OG	2.11	0.51
1:A:17:VAL:HG13	1:A:145:HIS:HB2	1.93	0.50
1:A:242:MET:O	1:A:243:LYS:HG3	2.11	0.50
1:A:98:THR:HG22	1:A:100:ASP:CB	2.41	0.50
1:A:227:ILE:O	1:A:227:ILE:HG13	2.11	0.50
2:B:1:CYS:HB2	2:B:14:GLU:CG	2.40	0.50
2:B:41:PRO:HB2	2:B:42:TYR:CD2	2.46	0.50
1:A:126:ASP:O	1:A:130:SER:HB3	2.11	0.50
1:A:202:ARG:HD2	1:A:207:TYR:CE1	2.47	0.49
1:A:202:ARG:HD2	1:A:207:TYR:CZ	2.47	0.49
1:A:32:LEU:HD11	1:A:40:GLY:HA3	1.93	0.49
1:A:247:LEU:HB3	1:A:248:PRO:HD3	1.94	0.49
1:A:153:THR:CB	3:A:794:HOH:O	2.60	0.49
1:A:124(A):GLU:OE2	2:B:11:PHE:CD2	2.66	0.49
2:B:1:CYS:HB2	2:B:14:GLU:HG2	1.94	0.49
2:B:1:CYS:H1	2:B:19:VAL:HG21	1.74	0.49
1:A:49:GLU:CD	1:A:49:GLU:H	2.17	0.48
2:B:13:HIS:O	2:B:20:VAL:N	2.45	0.48
1:A:23:LYS:HG2	1:A:26:GLU:OE2	2.11	0.48
1:A:246:GLY:O	1:A:247:LEU:HD12	2.13	0.48
1:A:58:CYS:O	1:A:61:GLN:CG	2.61	0.48
1:A:34:ILE:CD1	1:A:67:ARG:HD3	2.42	0.48
1:A:62:LYS:HB2	1:A:62:LYS:NZ	2.27	0.48
1:A:236:LYS:O	1:A:239:ASP:HB2	2.13	0.48
1:A:71:ARG:O	1:A:155:LEU:N	2.45	0.48
1:A:165:ARG:NH2	1:A:178:GLN:HA	2.29	0.48
1:A:127:TRP:HZ2	1:A:203:PHE:CE2	2.32	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:13:HIS:O	2:B:20:VAL:HG13	2.14	0.47
1:A:115:ARG:CZ	1:A:118:VAL:HG21	2.44	0.47
1:A:211:GLY:HA2	1:A:229:THR:O	2.15	0.47
1:A:244:THR:HA	3:A:798:HOH:O	2.13	0.47
1:A:135:THR:CG2	1:A:159:GLU:HG3	2.44	0.47
1:A:103:ILE:HD13	1:A:234:PHE:CB	2.45	0.47
1:A:175:ILE:HD13	1:A:175:ILE:HG21	1.51	0.47
1:A:58:CYS:O	1:A:61:GLN:HG2	2.15	0.47
1:A:47:LEU:HD11	1:A:53:LEU:HB2	1.97	0.47
2:B:14:GLU:CA	2:B:18:SER:O	2.60	0.46
1:A:75:GLN:HB3	1:A:75:GLN:HE21	1.55	0.46
1:A:108:LEU:HD11	1:A:112:ILE:HD11	1.96	0.46
2:B:16:GLN:O	2:B:17:ASN:HB3	2.15	0.46
2:B:26:GLY:O	3:B:605:HOH:O	2.21	0.46
1:A:60:TYR:CE2	1:A:96:LYS:HE3	2.51	0.46
1:A:134:LYS:HB3	1:A:134:LYS:HE2	1.73	0.46
1:A:145:HIS:C	3:A:527:HOH:O	2.55	0.45
1:A:240:ARG:O	1:A:244:THR:HG22	2.17	0.45
1:A:113:THR:HG23	3:A:776:HOH:O	2.15	0.45
1:A:79:GLY:HA3	3:A:712:HOH:O	2.11	0.45
2:B:38:PRO:CB	2:B:43:PRO:HG3	2.47	0.45
1:A:25:GLY:O	2:B:47:GLN:HB3	2.17	0.44
2:B:10:GLN:OE1	2:B:24:ALA:CB	2.66	0.44
1:A:59:LEU:HD12	1:A:90:LYS:HG3	1.99	0.44
1:A:109:LYS:O	1:A:110:THR:HG23	2.16	0.44
1:A:222:ARG:HG3	3:A:545:HOH:O	2.18	0.44
1:A:136:GLY:HA3	1:A:199:HIS:CE1	2.53	0.44
1:A:127:TRP:CZ2	1:A:203:PHE:CD2	3.05	0.44
1:A:17:VAL:CG1	1:A:145:HIS:HB2	2.48	0.43
2:B:29:LEU:HD21	2:B:33:GLY:O	2.18	0.43
1:A:236:LYS:O	1:A:239:ASP:CB	2.66	0.43
2:B:15:GLU:O	2:B:16:GLN:C	2.57	0.43
1:A:78:GLY:C	1:A:80:GLU:H	2.22	0.43
2:B:29:LEU:HA	2:B:35:ALA:O	2.19	0.42
1:A:239:ASP:O	1:A:242:MET:N	2.52	0.42
2:B:38:PRO:HB3	2:B:43:PRO:HG3	2.00	0.42
1:A:23:LYS:HZ2	1:A:23:LYS:HB3	1.85	0.42
1:A:23:LYS:C	1:A:71:ARG:NH1	2.72	0.42
1:A:247:LEU:HB3	1:A:248:PRO:CD	2.49	0.42
1:A:165:ARG:O	1:A:168:CYS:HB3	2.19	0.42
1:A:95:THR:HG22	1:A:97:GLU:HG2	2.01	0.42
1:A:23:LYS:C	1:A:71:ARG:HH11	2.22	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:SER:O	1:A:132:THR:CB	2.68	0.42
1:A:187:GLN:HA	1:A:221:ALA:HB1	2.01	0.42
2:B:13:HIS:HE1	3:B:510:HOH:O	1.87	0.42
1:A:65:LYS:HE2	1:A:84:GLU:HG2	2.02	0.42
1:A:70:ASP:O	1:A:141:PHE:HZ	2.02	0.42
1:A:33:LEU:N	1:A:33:LEU:HD23	2.35	0.42
2:B:5:ASN:C	2:B:7:ASP:N	2.72	0.42
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.95	0.42
2:B:19:VAL:HG12	2:B:19:VAL:O	2.19	0.42
2:B:32:ASN:OD1	2:B:33:GLY:N	2.53	0.42
1:A:41:PHE:CE2	1:A:61(A):ALA:HB2	2.55	0.42
1:A:176:ILE:HA	1:A:176:ILE:HD13	1.87	0.41
1:A:130:SER:O	1:A:132:THR:HB	2.20	0.41
1:A:107:ARG:HD2	1:A:107:ARG:HH11	1.61	0.41
1:A:72:ASN:HA	1:A:154:ARG:HA	2.03	0.41
1:A:23:LYS:NZ	1:A:23:LYS:HB3	2.36	0.41
1:A:121:ALA:HB1	1:A:209:VAL:HG22	2.02	0.41
2:B:29:LEU:HD12	2:B:35:ALA:H	1.86	0.40
1:A:124:PRO:HB2	1:A:128:ALA:HB2	2.04	0.40
1:A:144:THR:O	1:A:145:HIS:CB	2.69	0.40
2:B:14:GLU:OE1	2:B:19:VAL:CG2	2.70	0.40
2:B:29:LEU:CD1	2:B:35:ALA:H	2.35	0.40
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.85	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	A	232/241 (96%)	203 (88%)	20 (9%)	9 (4%)	5	2
2	B	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	11	6
All	All	281/292 (96%)	249 (89%)	22 (8%)	10 (4%)	5	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY
1	A	77	GLU
1	A	247	LEU
1	A	23	LYS
1	A	59	LEU
1	A	73	THR
1	A	74	GLU
2	B	3	LEU
1	A	36	GLU
1	A	182	CYS

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	A	200/204 (98%)	153 (76%)	47 (24%)	1	0
2	B	43/43 (100%)	32 (74%)	11 (26%)	1	0
All	All	243/247 (98%)	185 (76%)	58 (24%)	1	0

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	24	ASP
1	A	33	LEU
1	A	36	GLU
1	A	62	LYS
1	A	63	ARG
1	A	67	ARG
1	A	70	ASP
1	A	73	THR
1	A	74	GLU
1	A	75	GLN
1	A	76	GLU
1	A	87	VAL
1	A	88	VAL
1	A	93	ARG
1	A	95	THR

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Mol	Chain	Res	Type
1	A	96	LYS
1	A	98	THR
1	A	106	LEU
1	A	116	MET
1	A	125	ARG
1	A	126	ASP
1	A	130	SER
1	A	133	GLN
1	A	134	LYS
1	A	135	THR
1	A	139	SER
1	A	145	HIS
1	A	153	THR
1	A	154	ARG
1	A	158	LEU
1	A	164	ASP
1	A	167	SER
1	A	170	LEU
1	A	178	GLN
1	A	181	PHE
1	A	185(B)	THR
1	A	192	GLN
1	A	200	VAL
1	A	227	ILE
1	A	232	THR
1	A	235	LEU
1	A	239	ASP
1	A	244	THR
1	A	247	LEU
1	A	249	LYS
1	A	251	LYS
2	B	1	CYS
2	B	7	ASP
2	B	17	ASN
2	B	18	SER
2	B	20	VAL
2	B	25	ARG
2	B	28	THR
2	B	31	ASP
2	B	38	PRO
2	B	39	THR
2	B	49	LEU

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	72	ASN
1	A	75	GLN
1	A	91	HIS
1	A	117	ASN
1	A	133	GLN
1	A	166	ASN
1	A	178	GLN

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 ⓘ

There are no ligands in this entry.

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.