



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:42 AM GMT

PDB ID : 2HGT
Title : STRUCTURE OF THE HIRUGEN AND HIRULOG 1 COMPLEXES OF
ALPHA-THROMBIN
Authors : Tulinsky, A.; Carperos, V.
Deposited on : 1991-06-03
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>

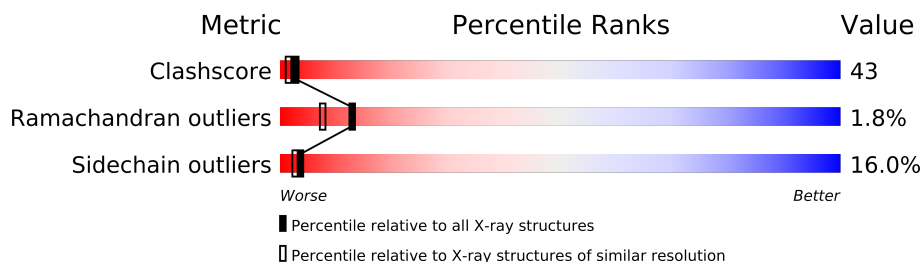
The following versions of software and data (see [references](#)) were used in the production of this report:

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	L	36	
2	H	259	
3	I	3	
4	J	17	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2616 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	33	Total	C	N	O	S	0	0	0
			265	162	45	57	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	253	Total	C	N	O	S	0	0	0
			2053	1310	362	367	14			

- Molecule 3 is a protein called Hirulog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			30	20	6	4			

- Molecule 4 is a protein called Hirulog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	6	Total	C	N	O	0	0	1
			46	29	6	11			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	188	Total	O	0	0
			188	188		
5	I	1	Total	O	0	0
			1	1		
5	J	4	Total	O	0	0
			4	4		
5	L	29	Total	O	0	0
			29	29		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.65Å 72.40Å 72.82Å 90.00° 100.76° 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	Depositor
R, R_{free}	0.163 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2616	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	L	1.16	0/267	3.15	18/353 (5.1%)
2	H	1.14	0/2107	2.24	89/2846 (3.1%)
3	I	1.56	0/19	2.15	2/22 (9.1%)
4	J	1.30	1/46 (2.2%)	2.28	3/61 (4.9%)
All	All	1.15	1/2439 (0.0%)	2.36	112/3282 (3.4%)

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	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	59	ILE	C-N	-5.07	1.24	1.34

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	15	ARG	CD-NE-CZ	24.99	158.59	123.60
1	L	15	ARG	NE-CZ-NH2	-22.33	109.13	120.30
1	L	15	ARG	NE-CZ-NH1	21.75	131.18	120.30
2	H	77(A)	ARG	NE-CZ-NH2	-17.67	111.47	120.30
2	H	233	ARG	NE-CZ-NH2	-16.56	112.02	120.30
2	H	101	ARG	NE-CZ-NH1	15.58	128.09	120.30
2	H	221(A)	ARG	NE-CZ-NH2	-12.67	113.96	120.30
2	H	233	ARG	NE-CZ-NH1	12.18	126.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75	ARG	NE-CZ-NH1	12.11	126.35	120.30
2	H	50	ARG	NE-CZ-NH1	11.83	126.22	120.30
2	H	202	LYS	CA-CB-CG	11.46	138.62	113.40
2	H	175	ARG	NE-CZ-NH2	-11.25	114.67	120.30
2	H	101	ARG	NE-CZ-NH2	-10.91	114.84	120.30
2	H	35	ARG	NE-CZ-NH2	-10.88	114.86	120.30
2	H	75	ARG	NE-CZ-NH2	-10.84	114.88	120.30
2	H	206	ARG	NE-CZ-NH2	-10.61	115.00	120.30
2	H	202	LYS	CB-CG-CD	10.01	137.63	111.60
2	H	206	ARG	NE-CZ-NH1	9.82	125.21	120.30
2	H	221(A)	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	H	50	ARG	NE-CZ-NH2	-9.58	115.51	120.30
2	H	187	ARG	NE-CZ-NH2	9.38	124.99	120.30
2	H	117	TYR	CB-CG-CD2	-9.27	115.44	121.00
1	L	14(K)	ILE	CB-CA-C	9.14	129.87	111.60
2	H	225	TYR	CB-CG-CD2	-8.90	115.66	121.00
2	H	178	ASP	CB-CG-OD2	-8.79	110.39	118.30
2	H	117	TYR	CB-CG-CD1	8.60	126.16	121.00
2	H	164	GLU	CA-CB-CG	8.46	132.01	113.40
2	H	186(C)	GLY	C-N-CA	8.37	142.62	121.70
2	H	175	ARG	NH1-CZ-NH2	8.35	128.58	119.40
2	H	116	ASP	CB-CG-OD1	7.95	125.45	118.30
2	H	194	ASP	CB-CG-OD1	-7.85	111.24	118.30
2	H	126	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	L	13	GLU	CA-CB-CG	7.67	130.26	113.40
2	H	165	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	H	225	TYR	CB-CG-CD1	7.44	125.46	121.00
2	H	184(A)	TYR	CB-CG-CD1	-7.39	116.56	121.00
2	H	77(A)	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	H	21	ASP	CB-CG-OD1	7.21	124.79	118.30
2	H	175	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	L	14	ASP	CB-CG-OD2	-7.11	111.90	118.30
2	H	154	VAL	N-CA-CB	-7.09	95.89	111.50
2	H	222	ASP	CB-CG-OD1	-7.07	111.94	118.30
2	H	77(A)	ARG	CA-C-O	-6.97	105.46	120.10
1	L	1(A)	ASP	CB-CG-OD1	-6.81	112.17	118.30
2	H	187	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	L	14(G)	LEU	CB-CA-C	6.67	122.88	110.20
2	H	42	CYS	N-CA-CB	-6.56	98.79	110.60
2	H	62	ASN	CB-CA-C	-6.54	97.33	110.40
2	H	81	LYS	N-CA-CB	6.53	122.35	110.60
1	L	14(M)	GLY	N-CA-C	6.51	129.38	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(K)	ILE	CA-C-O	6.50	133.74	120.10
2	H	165	ARG	CD-NE-CZ	-6.44	114.58	123.60
2	H	21	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	H	91	HIS	CA-CB-CG	-6.35	102.81	113.60
2	H	208	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	H	20	SER	O-C-N	6.29	132.76	122.70
2	H	39	GLU	OE1-CD-OE2	6.22	130.77	123.30
2	H	148	TRP	CA-CB-CG	-6.22	101.87	113.70
2	H	38	GLN	O-C-N	6.18	132.58	122.70
2	H	60(E)	ASP	CB-CG-OD1	-6.16	112.76	118.30
2	H	204(B)	ASN	C-N-CA	6.13	137.02	121.70
4	J	58	GLU	CG-CD-OE1	6.12	130.54	118.30
2	H	170	ASP	CA-CB-CG	-6.09	100.00	113.40
2	H	114	PHE	CB-CG-CD1	-6.07	116.55	120.80
2	H	163	VAL	CA-CB-CG1	6.02	119.93	110.90
2	H	233	ARG	CD-NE-CZ	6.02	132.03	123.60
2	H	27	SER	N-CA-CB	-5.95	101.58	110.50
2	H	64	LEU	N-CA-C	5.92	126.99	111.00
2	H	27	SER	CB-CA-C	5.82	121.16	110.10
2	H	190	ALA	N-CA-C	-5.78	95.39	111.00
2	H	84	MET	CA-CB-CG	-5.77	103.50	113.30
2	H	175	ARG	CD-NE-CZ	5.73	131.62	123.60
2	H	147	THR	N-CA-CB	5.72	121.17	110.30
2	H	93	ARG	NE-CZ-NH2	5.72	123.16	120.30
2	H	232	PHE	CB-CG-CD1	-5.69	116.82	120.80
1	L	14(J)	TYR	CA-C-N	-5.68	104.71	117.20
3	I	3	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	L	8	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	L	1(C)	GLU	CG-CD-OE1	-5.64	107.02	118.30
2	H	77(A)	ARG	CA-C-N	5.64	129.60	117.20
2	H	47	ILE	CB-CG1-CD1	5.62	129.62	113.90
2	H	84	MET	CA-C-N	-5.58	104.91	117.20
2	H	65	LEU	CB-CG-CD2	-5.58	101.51	111.00
2	H	181	PHE	N-CA-CB	5.52	120.54	110.60
2	H	232	PHE	CA-CB-CG	-5.49	100.72	113.90
2	H	175	ARG	CG-CD-NE	-5.48	100.28	111.80
2	H	183	ALA	C-N-CA	5.48	133.80	122.30
1	L	1(B)	ALA	CA-C-O	5.47	131.59	120.10
2	H	129(C)	LEU	O-C-N	5.47	131.46	122.70
2	H	93	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	H	60(A)	TYR	CB-CG-CD1	-5.45	117.73	121.00
3	I	3	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	ASN	OD1-CG-ND2	5.41	134.34	121.90
1	L	14(C)	GLU	CG-CD-OE2	5.39	129.08	118.30
2	H	48	SER	O-C-N	5.38	131.31	122.70
4	J	58	GLU	CG-CD-OE2	-5.38	107.55	118.30
2	H	116	ASP	CB-CG-OD2	-5.34	113.49	118.30
2	H	40	LEU	O-C-N	5.32	131.21	122.70
1	L	14(D)	ARG	CD-NE-CZ	5.29	131.00	123.60
4	J	58	GLU	CB-CG-CD	5.28	128.45	114.20
2	H	97	ARG	CD-NE-CZ	-5.25	116.25	123.60
2	H	66	VAL	CA-CB-CG1	5.21	118.72	110.90
2	H	103	ILE	O-C-N	5.20	131.02	122.70
2	H	165	ARG	NE-CZ-NH1	-5.17	117.72	120.30
2	H	164	GLU	CB-CG-CD	5.14	128.08	114.20
2	H	20	SER	CB-CA-C	-5.10	100.42	110.10
2	H	199	PHE	CB-CA-C	5.08	120.56	110.40
1	L	14(M)	GLY	CA-C-O	5.07	129.73	120.60
2	H	74	THR	OG1-CB-CG2	5.05	121.61	110.00
2	H	18	GLU	CG-CD-OE2	5.03	128.37	118.30
2	H	192	GLU	CA-CB-CG	5.00	124.41	113.40
1	L	2	GLY	CA-C-O	-5.00	111.60	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	165	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	L	265	0	259	29	4
2	H	2053	0	2020	187	3
3	I	30	0	30	1	0
4	J	46	0	35	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	188	0	0	22	0
5	I	1	0	0	0	0
5	J	4	0	0	1	0
5	L	29	0	0	5	0
All	All	2616	0	2344	205	4

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 43.

All (205) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:236:LYS:HA	2:H:239:GLN:NE2	1.44	1.31
2:H:201:MET:HE3	2:H:210:MET:CG	1.73	1.18
2:H:124:PRO:HG3	2:H:210:MET:HE2	1.28	1.11
2:H:128:THR:HG23	5:H:626:HOH:O	1.54	1.07
2:H:201:MET:CE	2:H:210:MET:HG3	1.85	1.06
2:H:147:THR:HA	2:H:148:TRP:CZ3	1.91	1.05
2:H:129(C):LEU:HD12	5:H:626:HOH:O	1.55	1.04
2:H:236:LYS:HA	2:H:239:GLN:HE22	1.01	1.01
2:H:35:ARG:O	2:H:38:GLN:HA	1.61	1.00
2:H:145:LYS:HB2	5:H:611:HOH:O	1.60	1.00
2:H:219:GLY:HA3	2:H:221(A):ARG:HD2	1.46	0.98
2:H:147:THR:CA	2:H:148:TRP:CE3	2.47	0.97
2:H:50:ARG:HG3	2:H:247:GLU:HG3	1.46	0.96
2:H:139:THR:HG22	2:H:157:VAL:HG12	1.47	0.96
2:H:199:PHE:CD2	5:H:638:HOH:O	2.18	0.96
2:H:110:LYS:HD3	5:H:559:HOH:O	1.63	0.96
2:H:147:THR:HA	2:H:148:TRP:CE3	1.99	0.95
2:H:201:MET:SD	5:H:642:HOH:O	2.25	0.94
2:H:50:ARG:CG	2:H:247:GLU:HG3	1.98	0.93
2:H:87:LYS:HD3	2:H:88:ILE:H	1.32	0.93
2:H:236:LYS:N	2:H:236:LYS:HD3	1.85	0.92
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.04	0.91
2:H:50:ARG:NH2	2:H:108:LEU:O	2.04	0.90
2:H:35:ARG:HB3	2:H:39:GLU:HG3	1.53	0.89
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.54	0.87
2:H:85:LEU:HD13	2:H:106:MET:CE	2.05	0.86
2:H:87:LYS:HD3	2:H:88:ILE:N	1.90	0.85
2:H:201:MET:HE3	2:H:210:MET:HG3	0.91	0.84
2:H:50:ARG:CB	2:H:247:GLU:HG3	2.07	0.84
1:L:15:ARG:HB2	2:H:204:PRO:O	1.77	0.84
2:H:50:ARG:HB2	2:H:247:GLU:HG3	1.58	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:148:TRP:CD2	2:H:148:TRP:N	2.49	0.80
2:H:50:ARG:NH2	2:H:86:GLU:OE1	2.12	0.79
1:L:1(C):GLU:HG3	2:H:48:SER:HA	1.64	0.79
1:L:1(D):GLY:HA3	2:H:122:CYS:HA	1.67	0.77
2:H:208:TYR:HB3	2:H:210:MET:HE3	1.65	0.77
2:H:147:THR:C	2:H:148:TRP:CE3	2.59	0.76
1:L:14(H):GLU:HA	1:L:14(L):ASP:HA	1.67	0.76
2:H:145:LYS:CG	2:H:148:TRP:HB3	2.15	0.75
2:H:50:ARG:NH2	2:H:107:LYS:HE2	2.01	0.75
2:H:81:LYS:HD2	2:H:118:ILE:CD1	2.17	0.75
2:H:37:PRO:O	2:H:39:GLU:HG2	1.87	0.75
2:H:124:PRO:CG	2:H:210:MET:HE2	2.12	0.74
2:H:147:THR:CA	2:H:148:TRP:CZ3	2.68	0.74
2:H:77:GLU:HB2	2:H:80:GLU:HG2	1.71	0.73
2:H:208:TYR:HB3	2:H:210:MET:CE	2.18	0.72
2:H:50:ARG:HB2	2:H:247:GLU:CG	2.19	0.72
1:L:1(C):GLU:N	5:L:416:HOH:O	2.18	0.71
2:H:145:LYS:CD	2:H:148:TRP:HB3	2.21	0.71
2:H:145:LYS:HD2	2:H:148:TRP:HB3	1.73	0.70
2:H:236:LYS:CA	2:H:239:GLN:NE2	2.40	0.70
1:L:14(I):SER:C	1:L:14(K):ILE:H	1.93	0.69
2:H:199:PHE:CE2	5:H:638:HOH:O	2.40	0.69
1:L:1(E):SER:HA	2:H:123:LEU:O	1.92	0.69
2:H:81:LYS:NZ	2:H:118:ILE:HD12	2.07	0.69
2:H:201:MET:CE	2:H:210:MET:CG	2.55	0.68
2:H:116:ASP:HB2	5:H:536:HOH:O	1.95	0.67
2:H:147:THR:HB	5:H:615:HOH:O	1.95	0.67
1:L:1(E):SER:CA	2:H:123:LEU:O	2.41	0.67
2:H:35:ARG:CB	2:H:39:GLU:HG3	2.24	0.67
2:H:17:VAL:O	2:H:188:GLY:HA2	1.94	0.67
2:H:35:ARG:HD3	2:H:39:GLU:OE2	1.94	0.67
2:H:50:ARG:CG	2:H:247:GLU:CG	2.72	0.66
2:H:35:ARG:O	2:H:38:GLN:CA	2.42	0.66
1:L:14(D):ARG:NH2	1:L:14(H):GLU:OE2	2.28	0.66
2:H:124:PRO:HG3	2:H:210:MET:CE	2.15	0.65
1:L:1(B):ALA:HB2	5:L:573:HOH:O	1.95	0.65
2:H:236:LYS:N	2:H:236:LYS:CD	2.58	0.65
2:H:36(A):SER:HA	2:H:37:PRO:C	2.17	0.65
2:H:81:LYS:HD2	2:H:118:ILE:HD12	1.78	0.65
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.62	0.65
2:H:81:LYS:HZ2	2:H:118:ILE:HD12	1.62	0.64
2:H:219:GLY:CA	2:H:221(A):ARG:HD2	2.26	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:236:LYS:HD3	2:H:236:LYS:H	1.62	0.63
1:L:1(D):GLY:CA	2:H:123:LEU:H	2.11	0.63
1:L:1(D):GLY:N	2:H:123:LEU:H	1.97	0.63
2:H:148:TRP:N	2:H:148:TRP:CE3	2.68	0.62
2:H:50:ARG:CB	2:H:247:GLU:CG	2.78	0.61
2:H:232:PHE:O	2:H:235:LYS:HB2	2.00	0.61
2:H:236:LYS:CA	2:H:239:GLN:HE22	1.94	0.61
2:H:145:LYS:HG3	2:H:148:TRP:HB3	1.82	0.61
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.37	0.60
2:H:191:CYS:O	2:H:194:ASP:HB2	2.03	0.59
2:H:146:GLU:HG3	5:H:493:HOH:O	2.01	0.59
2:H:124:PRO:HB3	2:H:210:MET:HE1	1.85	0.58
2:H:182:CYS:HA	2:H:226:GLY:O	2.03	0.58
2:H:35:ARG:NH2	5:H:491:HOH:O	2.36	0.58
2:H:50:ARG:HG3	2:H:247:GLU:CG	2.26	0.58
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.34	0.58
2:H:204(B):ASN:HD22	2:H:204(B):ASN:C	2.08	0.58
2:H:145:LYS:HB2	2:H:148:TRP:CE3	2.39	0.57
4:J:57:GLU:HA	5:J:561:HOH:O	2.02	0.57
2:H:126:ARG:HB3	2:H:127:GLU:OE1	2.04	0.57
2:H:85:LEU:CD1	2:H:106:MET:CE	2.82	0.56
1:L:1(E):SER:HB2	2:H:123:LEU:O	2.05	0.56
2:H:18:GLU:HA	2:H:18:GLU:OE1	2.06	0.55
2:H:60(F):LYS:HB2	5:H:614:HOH:O	2.06	0.55
2:H:77(A):ARG:HD3	5:H:572:HOH:O	2.06	0.55
2:H:17:VAL:O	2:H:18:GLU:HB2	2.06	0.55
2:H:50:ARG:HH21	2:H:107:LYS:HE2	1.70	0.55
2:H:162:ILE:CD1	2:H:199:PHE:CZ	2.90	0.55
2:H:50:ARG:CZ	2:H:108:LEU:O	2.54	0.55
4:J:57:GLU:HG3	4:J:58:GLU:N	2.21	0.54
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.08	0.54
2:H:241:VAL:HA	2:H:244:GLN:HE21	1.72	0.54
4:J:57:GLU:CG	4:J:58:GLU:N	2.70	0.54
2:H:50:ARG:NH1	5:H:503:HOH:O	2.40	0.54
2:H:239:GLN:HA	5:H:643:HOH:O	2.07	0.53
2:H:69:GLY:O	2:H:79:ILE:HD11	2.07	0.53
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.91	0.53
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	2.09	0.53
2:H:89:TYR:CE2	2:H:245:PHE:CE1	2.97	0.52
2:H:204(B):ASN:HD22	2:H:205:ASN:N	2.06	0.52
2:H:97:ARG:HH11	2:H:97:ARG:HG2	1.74	0.52
2:H:236:LYS:HA	2:H:239:GLN:HE21	1.61	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:14(D):ARG:HB2	5:L:421:HOH:O	2.09	0.52
2:H:129:ALA:O	2:H:130:LEU:HB2	2.10	0.52
2:H:219:GLY:HA3	2:H:221(A):ARG:CD	2.32	0.51
2:H:165:ARG:N	2:H:166:PRO:HD2	2.24	0.51
2:H:99:LEU:HD11	3:I:2:PRO:HB3	1.91	0.51
2:H:50:ARG:HD2	2:H:111:PRO:HD3	1.91	0.51
2:H:236:LYS:HD2	2:H:239:GLN:HE22	1.75	0.51
2:H:86:GLU:HB2	2:H:109:LYS:HA	1.93	0.51
2:H:50:ARG:HD2	2:H:111:PRO:CD	2.41	0.50
2:H:110:LYS:HG3	2:H:111:PRO:HD2	1.93	0.50
1:L:1(E):SER:CB	2:H:123:LEU:O	2.60	0.50
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.94	0.50
2:H:162:ILE:CD1	2:H:199:PHE:HZ	2.24	0.50
2:H:186(C):GLY:O	5:H:645:HOH:O	2.19	0.50
2:H:38:GLN:HE22	4:J:59:ILE:HG23	1.78	0.49
2:H:145:LYS:HD2	2:H:148:TRP:CB	2.42	0.49
2:H:110:LYS:CG	2:H:111:PRO:HD2	2.42	0.49
1:L:1(D):GLY:CA	5:L:416:HOH:O	2.61	0.49
2:H:51:TRP:HE1	2:H:247:GLU:H	1.61	0.49
2:H:35:ARG:CD	2:H:39:GLU:OE2	2.61	0.48
2:H:84:MET:O	2:H:109:LYS:HB2	2.12	0.48
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.48	0.48
2:H:97:ARG:NH1	2:H:97:ARG:HG2	2.28	0.48
1:L:14(A):LYS:HE3	1:L:14(B):THR:HG23	1.96	0.48
2:H:186(B):GLU:O	2:H:186(C):GLY:C	2.52	0.48
2:H:208:TYR:HB3	2:H:210:MET:HE1	1.96	0.47
1:L:10:LYS:NZ	5:L:489:HOH:O	2.46	0.47
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.48	0.47
2:H:203:SER:O	2:H:205:ASN:HA	2.14	0.47
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.67	0.47
2:H:134:TYR:CD1	2:H:134:TYR:N	2.83	0.47
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.96	0.47
1:L:15:ARG:HG2	1:L:15:ARG:O	2.15	0.46
2:H:75:ARG:H	2:H:75:ARG:HG3	1.45	0.46
2:H:134:TYR:HD1	2:H:134:TYR:N	2.13	0.46
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.45	0.46
2:H:236:LYS:CD	2:H:239:GLN:HE22	2.28	0.46
2:H:241:VAL:HB	2:H:245:PHE:HE1	1.80	0.46
2:H:221(A):ARG:HG3	5:H:402:HOH:O	2.16	0.46
2:H:59:LEU:O	2:H:60(F):LYS:HG2	2.16	0.46
2:H:145:LYS:O	2:H:148:TRP:CZ3	2.69	0.46
2:H:49:ASP:HB2	2:H:112:VAL:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.63	0.45
2:H:20:SER:O	2:H:157:VAL:N	2.48	0.45
2:H:165:ARG:HG3	5:H:557:HOH:O	2.17	0.45
1:L:14(G):LEU:HD21	2:H:202:LYS:HG3	1.99	0.45
2:H:217:GLU:OE1	2:H:224:LYS:NZ	2.47	0.45
2:H:65:LEU:HD11	2:H:84:MET:CE	2.46	0.44
2:H:244:GLN:HG2	2:H:245:PHE:CE2	2.52	0.44
2:H:236:LYS:CG	2:H:239:GLN:HE22	2.29	0.44
2:H:36(A):SER:HA	2:H:38:GLN:N	2.32	0.44
1:L:9:LYS:NZ	2:H:119:HIS:CE1	2.85	0.44
2:H:191:CYS:N	2:H:194:ASP:OD2	2.51	0.44
2:H:87:LYS:HB3	2:H:89:TYR:CE1	2.53	0.44
2:H:145:LYS:CB	2:H:148:TRP:HE3	2.30	0.43
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.99	0.43
2:H:127:GLU:HG2	5:H:546:HOH:O	2.19	0.43
2:H:127:GLU:CD	2:H:127:GLU:H	2.22	0.43
2:H:145:LYS:CB	2:H:148:TRP:CE3	3.02	0.43
2:H:58:CYS:O	2:H:60(F):LYS:HD3	2.19	0.43
2:H:165:ARG:HH11	2:H:165:ARG:HD3	1.58	0.43
2:H:145:LYS:N	5:H:611:HOH:O	2.51	0.43
2:H:239:GLN:HE21	2:H:239:GLN:HB2	1.40	0.42
2:H:81:LYS:CD	2:H:118:ILE:HD12	2.46	0.42
2:H:87:LYS:NZ	2:H:88:ILE:O	2.45	0.42
2:H:33:LEU:CD2	2:H:64:LEU:HD22	2.49	0.42
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.81	0.42
1:L:6:LEU:HA	1:L:10:LYS:HD2	2.02	0.42
2:H:60(F):LYS:HG3	2:H:60(H):PHE:CE2	2.55	0.42
2:H:119:HIS:HA	2:H:120:PRO:HD3	1.95	0.42
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.67	0.42
2:H:187:ARG:HH11	2:H:187:ARG:HD3	1.60	0.41
2:H:99:LEU:HD12	2:H:215:TRP:HB3	2.00	0.41
2:H:66:VAL:O	2:H:82:ILE:HA	2.20	0.41
2:H:65:LEU:HD11	2:H:84:MET:HE2	2.01	0.41
2:H:124:PRO:HB3	2:H:210:MET:CE	2.50	0.41
1:L:1(A):ASP:OD2	1:L:9:LYS:HE3	2.20	0.41
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE2	2.68	0.41
2:H:134:TYR:HB3	5:H:642:HOH:O	2.19	0.41
2:H:87:LYS:CD	2:H:88:ILE:O	2.69	0.41
2:H:77:GLU:CB	2:H:80:GLU:HG2	2.47	0.41
1:L:9:LYS:HZ1	2:H:119:HIS:CE1	2.39	0.41
2:H:16:ILE:N	2:H:194:ASP:OD2	2.54	0.41
2:H:167:VAL:HG11	2:H:185:LYS:HE2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.36	0.41
2:H:230:HIS:HB3	2:H:233:ARG:HB2	2.03	0.41
2:H:198:PRO:HB2	2:H:200:VAL:HG13	2.02	0.41
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.18	0.41
1:L:14(G):LEU:O	1:L:14(M):GLY:N	2.54	0.41
2:H:151:GLN:HB3	5:H:495:HOH:O	2.20	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:15:ARG:NH2	2:H:169:LYS:O[4_556]	1.73	0.47
1:L:14(M):GLY:O	2:H:173:ARG:NE[4_556]	2.12	0.08
1:L:15:ARG:CZ	2:H:172:THR:O[4_556]	2.17	0.03
1:L:14(H):GLU:OE2	1:L:14(L):ASP:OD2[2_556]	2.19	0.01

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	L	31/36 (86%)	24 (77%)	4 (13%)	3 (10%)	1	0
2	H	249/259 (96%)	232 (93%)	15 (6%)	2 (1%)	27	24
3	I	1/3 (33%)	1 (100%)	0	0	100	100
4	J	4/17 (24%)	4 (100%)	0	0	100	100
All	All	285/315 (90%)	261 (92%)	19 (7%)	5 (2%)	13	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(M)	GLY
1	L	1(B)	ALA
2	H	186(C)	GLY
2	H	186(B)	GLU
1	L	14(L)	ASP

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	L	29/31 (94%)	21 (72%)	8 (28%)	0	0
2	H	221/225 (98%)	190 (86%)	31 (14%)	5	4
3	I	2/2 (100%)	2 (100%)	0	100	100
4	J	5/12 (42%)	3 (60%)	2 (40%)	0	0
All	All	257/270 (95%)	216 (84%)	41 (16%)	3	3

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	9	LYS
1	L	10	LYS
1	L	14	ASP
1	L	14(A)	LYS
1	L	14(D)	ARG
1	L	14(K)	ILE
1	L	14(L)	ASP
2	H	33	LEU
2	H	36	LYS
2	H	41	LEU
2	H	46	LEU
2	H	60(I)	THR
2	H	65	LEU
2	H	74	THR
2	H	79	ILE
2	H	83	SER
2	H	84	MET
2	H	107	LYS
2	H	109	LYS
2	H	110	LYS
2	H	125	ASP
2	H	127	GLU
2	H	130	LEU
2	H	151	GLN
2	H	154	VAL

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Mol	Chain	Res	Type
2	H	164	GLU
2	H	169	LYS
2	H	186(A)	ASP
2	H	187	ARG
2	H	202	LYS
2	H	204(B)	ASN
2	H	205	ASN
2	H	235	LYS
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
2	H	243	ASP
2	H	245	PHE
4	J	58	GLU
4	J	59	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	62	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN
2	H	239	GLN
2	H	244	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DPN	I	1	3	11,11,12	5.51	2 (18%)	11,13,15	1.82	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DPN	I	1	3	-	0/4/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	DPN	O-C	17.83	1.23	1.11
3	I	1	DPN	CA-C	2.71	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	DPN	C-CA-N	-4.23	109.61	113.83
3	I	1	DPN	CZ-CE1-CD1	2.33	124.05	120.17
3	I	1	DPN	CE2-CZ-CE1	-2.17	115.45	119.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.