Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:47 AM BST

PDB ID	:	4HTC
Title	:	THE REFINED STRUCTURE OF THE HIRUDIN-THROMBIN COMPLEX
Authors	:	Tulinsky, A.; Rydel, T.J.; Bode, W.; Huber, R.
Deposited on	:	1993-06-25
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

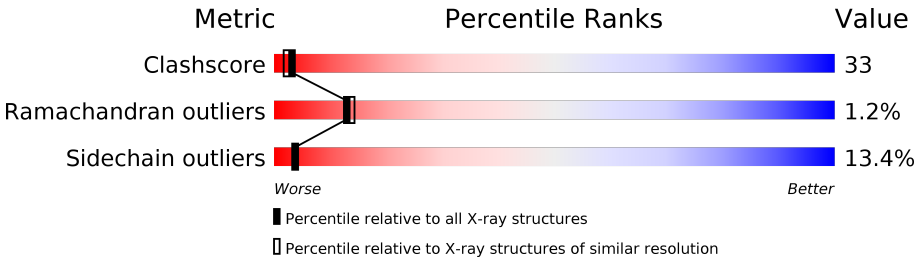
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	33% 42% 8% 8% 8%
2	H	259	48% 33% 15% .
3	I	65	31% 40% 12% 11% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	H	400	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			253	158	41	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	1
			2069	1323	366	366	14			

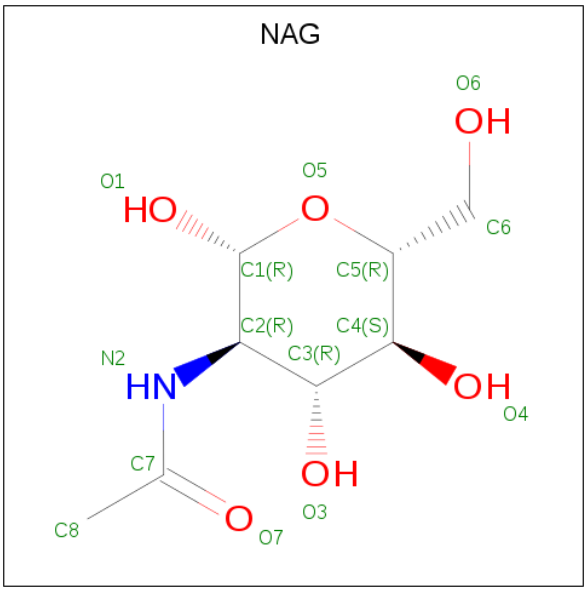
- Molecule 3 is a protein called HIRUDIN VARIANT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	61	Total	C	N	O	S	0	0	0
			447	267	75	99	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	47	LYS	ASN	conflict	UNP P09945

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	18	Total	O	0	0
			18	18		
5	H	199	Total	O	0	0
			199	199		
5	I	45	Total	O	0	0
			45	45		

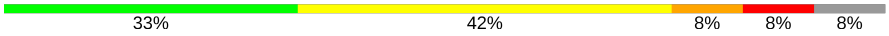
3 Residue-property plots (i)

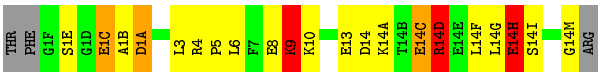
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: ALPHA-THROMBIN (SMALL SUBUNIT)

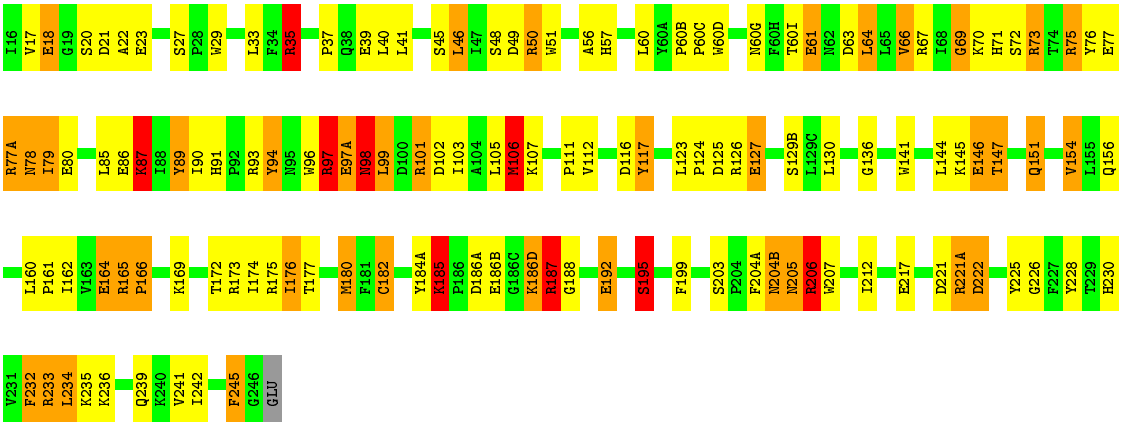
Chain L:





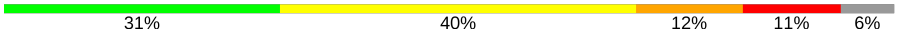
- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H:



- Molecule 3: HIRUDIN VARIANT 2

Chain I:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.54Å 90.54Å 132.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3045	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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: NAG

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	1.24	1/255 (0.4%)	2.52	15/338 (4.4%)
2	H	1.22	1/2124 (0.0%)	2.42	91/2872 (3.2%)
3	I	1.18	0/452	2.19	17/607 (2.8%)
All	All	1.22	2/2831 (0.1%)	2.40	123/3817 (3.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	195	SER	CA-CB	7.63	1.64	1.52
1	L	14(C)	GLU	CD-OE2	-5.60	1.19	1.25

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	73	ARG	NE-CZ-NH2	-25.25	107.67	120.30
2	H	35	ARG	NE-CZ-NH1	24.98	132.79	120.30
2	H	73	ARG	NE-CZ-NH1	24.86	132.73	120.30
2	H	175	ARG	NE-CZ-NH1	24.58	132.59	120.30
2	H	77(A)	ARG	NE-CZ-NH1	22.86	131.73	120.30
2	H	175	ARG	NE-CZ-NH2	-17.94	111.33	120.30
2	H	206	ARG	NE-CZ-NH1	-16.76	111.92	120.30
1	L	14(D)	ARG	NE-CZ-NH1	15.93	128.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	221(A)	ARG	NE-CZ-NH2	12.10	126.35	120.30
1	L	14(D)	ARG	NE-CZ-NH2	-11.80	114.40	120.30
2	H	206	ARG	NE-CZ-NH2	11.31	125.95	120.30
2	H	175	ARG	CD-NE-CZ	10.95	138.93	123.60
2	H	35	ARG	NE-CZ-NH2	-10.91	114.84	120.30
3	I	61	GLU	OE1-CD-OE2	9.85	135.12	123.30
2	H	165	ARG	NE-CZ-NH2	-9.82	115.39	120.30
3	I	3	TYR	CB-CG-CD1	-9.44	115.34	121.00
2	H	151	GLN	CA-CB-CG	9.41	134.10	113.40
2	H	77(A)	ARG	NE-CZ-NH2	-9.34	115.63	120.30
2	H	233	ARG	CD-NE-CZ	-9.34	110.53	123.60
2	H	221(A)	ARG	CD-NE-CZ	9.29	136.61	123.60
1	L	14(C)	GLU	OE1-CD-OE2	9.04	134.15	123.30
1	L	14(H)	GLU	OE1-CD-OE2	9.04	134.15	123.30
2	H	222	ASP	CB-CG-OD1	9.03	126.42	118.30
2	H	77(A)	ARG	CD-NE-CZ	8.72	135.80	123.60
2	H	212	ILE	O-C-N	8.48	136.27	122.70
2	H	187	ARG	NE-CZ-NH1	-8.46	116.07	120.30
2	H	192	GLU	OE1-CD-OE2	8.32	133.29	123.30
2	H	146	GLU	CG-CD-OE2	-8.18	101.94	118.30
2	H	35	ARG	CD-NE-CZ	8.05	134.87	123.60
2	H	101	ARG	CD-NE-CZ	-7.80	112.67	123.60
2	H	101	ARG	NE-CZ-NH1	-7.65	116.48	120.30
3	I	7	THR	CA-CB-CG2	7.61	123.06	112.40
2	H	245	PHE	O-C-N	7.44	135.84	123.20
1	L	14(H)	GLU	CG-CD-OE2	-7.33	103.64	118.30
2	H	67	ARG	NE-CZ-NH2	7.24	123.92	120.30
3	I	26	ASN	N-CA-CB	7.19	123.55	110.60
1	L	4	ARG	CD-NE-CZ	7.11	133.56	123.60
2	H	127	GLU	OE1-CD-OE2	-7.09	114.79	123.30
2	H	73	ARG	CG-CD-NE	-7.04	97.01	111.80
2	H	154	VAL	CA-CB-CG1	6.96	121.33	110.90
2	H	101	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	H	245	PHE	N-CA-CB	6.88	122.98	110.60
2	H	94	TYR	CB-CG-CD2	-6.85	116.89	121.00
2	H	27	SER	N-CA-CB	-6.80	100.30	110.50
2	H	185	LYS	CA-CB-CG	-6.75	98.54	113.40
1	L	9	LYS	CA-CB-CG	6.73	128.21	113.40
2	H	146	GLU	OE1-CD-OE2	6.68	131.32	123.30
2	H	61	GLU	CA-CB-CG	6.65	128.02	113.40
2	H	78	ASN	CB-CG-OD1	-6.53	108.55	121.60
2	H	151	GLN	N-CA-CB	6.44	122.19	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	35	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
2	H	233	ARG	CG-CD-NE	6.40	125.25	111.80
2	H	77(A)	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
2	H	123	LEU	CB-CA-C	6.32	122.21	110.20
1	L	1(A)	ASP	N-CA-CB	-6.31	99.24	110.60
2	H	77	GLU	C-N-CA	6.29	137.42	121.70
2	H	86	GLU	CG-CD-OE2	6.26	130.83	118.30
2	H	232	PHE	CB-CG-CD1	-6.26	116.42	120.80
2	H	101	ARG	NH1-CZ-NH2	6.23	126.25	119.40
3	I	61	GLU	CG-CD-OE1	-6.23	105.84	118.30
2	H	147	THR	CA-CB-CG2	6.21	121.09	112.40
2	H	89	TYR	CB-CG-CD2	-6.17	117.30	121.00
2	H	116	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	L	8	GLU	OE1-CD-OE2	6.11	130.63	123.30
2	H	97	ARG	CA-C-O	6.10	132.91	120.10
2	H	204(A)	PHE	CA-C-O	-6.10	107.29	120.10
1	L	13	GLU	CG-CD-OE2	6.08	130.46	118.30
1	L	13	GLU	OE1-CD-OE2	-6.08	116.01	123.30
2	H	180	MET	CB-CA-C	-6.06	98.29	110.40
2	H	186(D)	LYS	N-CA-CB	6.05	121.50	110.60
1	L	14(C)	GLU	CB-CA-C	-6.04	98.32	110.40
3	I	29	ILE	O-C-N	5.91	132.16	122.70
2	H	195	SER	CA-CB-OG	-5.87	95.34	111.20
2	H	75	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	H	98	ASN	N-CA-CB	5.81	121.06	110.60
2	H	94	TYR	CB-CG-CD1	5.81	124.49	121.00
2	H	127	GLU	CB-CA-C	5.77	121.94	110.40
2	H	204(A)	PHE	CB-CG-CD1	-5.76	116.77	120.80
2	H	117	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	L	14(C)	GLU	CG-CD-OE1	-5.74	106.81	118.30
3	I	21	VAL	CB-CA-C	-5.69	100.59	111.40
2	H	221	ASP	CB-CG-OD2	-5.66	113.20	118.30
3	I	38	GLN	O-C-N	5.62	131.69	122.70
2	H	106	MET	CA-CB-CG	5.55	122.74	113.30
2	H	73	ARG	O-C-N	-5.54	113.83	122.70
2	H	66	VAL	CB-CA-C	5.54	121.92	111.40
2	H	164	GLU	OE1-CD-OE2	-5.52	116.68	123.30
2	H	87	LYS	O-C-N	5.49	131.48	122.70
3	I	55	ASP	N-CA-CB	-5.48	100.73	110.60
2	H	76	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	H	205	ASN	CB-CG-OD1	-5.43	110.74	121.60
3	I	58	GLU	CB-CA-C	-5.42	99.56	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	180	MET	O-C-N	5.40	131.34	122.70
2	H	18	GLU	CB-CG-CD	-5.39	99.64	114.20
2	H	195	SER	CB-CA-C	-5.33	99.96	110.10
3	I	15	LEU	CB-CA-C	5.33	120.33	110.20
3	I	9	SER	CB-CA-C	5.28	120.13	110.10
3	I	11	GLN	N-CA-CB	5.28	120.10	110.60
1	L	13	GLU	CA-CB-CG	5.27	124.99	113.40
2	H	147	THR	N-CA-CB	5.25	120.28	110.30
2	H	79	ILE	CA-CB-CG1	-5.23	101.07	111.00
2	H	117	TYR	CB-CA-C	-5.21	99.99	110.40
2	H	186(A)	ASP	O-C-N	5.19	131.00	122.70
2	H	176	ILE	CB-CA-C	5.18	121.96	111.60
2	H	127	GLU	CG-CD-OE1	5.17	128.64	118.30
3	I	57	GLU	N-CA-CB	5.17	119.91	110.60
2	H	212	ILE	CA-C-O	-5.16	109.27	120.10
1	L	14(H)	GLU	CB-CA-C	-5.13	100.14	110.40
2	H	172	THR	CA-CB-CG2	5.13	119.58	112.40
2	H	125	ASP	CB-CG-OD1	5.12	122.90	118.30
3	I	65	GLN	CG-CD-NE2	-5.09	104.47	116.70
2	H	205	ASN	OD1-CG-ND2	5.09	133.61	121.90
3	I	3	TYR	CB-CG-CD2	5.09	124.05	121.00
2	H	98	ASN	O-C-N	5.06	130.79	122.70
2	H	40	LEU	CB-CA-C	5.04	119.77	110.20
2	H	233	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	H	166	PRO	O-C-N	5.03	130.75	122.70
2	H	145	LYS	CD-CE-NZ	-5.03	100.13	111.70
3	I	17	GLU	OE1-CD-OE2	5.03	129.33	123.30
2	H	245	PHE	N-CA-C	-5.02	97.45	111.00
2	H	69	GLY	C-N-CA	5.01	134.24	121.70
2	H	60(I)	THR	CA-CB-CG2	-5.01	105.39	112.40
2	H	63	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	206	ARG	Sidechain

5.2 Too-close contacts (i)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	253	0	244	18	1
2	H	2069	0	2040	116	1
3	I	447	0	399	61	0
4	H	14	0	13	2	0
5	H	199	0	0	21	0
5	I	45	0	0	14	0
5	L	18	0	0	5	0
All	All	3045	0	2696	183	1

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 33.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:452:HOH:O	3:I:53:ASN:HB3	1.26	1.28
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.33	1.09
3:I:58:GLU:CG	3:I:58:GLU:O	2.08	1.01
3:I:58:GLU:O	3:I:58:GLU:HG2	1.22	1.01
3:I:40:VAL:HG23	3:I:41:THR:O	1.60	1.00
1:L:14(M):GLY:HA3	5:L:603:HOH:O	1.58	0.99
3:I:13:LEU:HD12	3:I:46:PRO:HB3	1.46	0.97
3:I:55:ASP:OD1	3:I:55:ASP:N	1.98	0.97
3:I:52:ASN:HA	5:I:691:HOH:O	1.71	0.90
5:H:452:HOH:O	3:I:53:ASN:CB	1.93	0.85
3:I:13:LEU:HD11	3:I:24:LYS:HE3	1.60	0.83
2:H:173:ARG:HD3	3:I:20:ASN:OD1	1.78	0.82
2:H:126:ARG:HD2	5:H:738:HOH:O	1.79	0.82
2:H:60(B):PRO:HG2	2:H:96:TRP:CE2	2.16	0.80
2:H:35:ARG:HH11	2:H:35:ARG:HG3	1.48	0.79
2:H:174:ILE:HD11	3:I:21:VAL:HG21	1.66	0.78
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.18	0.77
2:H:165:ARG:NH1	2:H:180:MET:O	2.18	0.77
3:I:27:LYS:HG3	3:I:40:VAL:HG22	1.65	0.77
2:H:35:ARG:HD2	2:H:37:PRO:O	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:ASN:N	5:H:596:HOH:O	1.65	0.76
5:H:663:HOH:O	3:I:53:ASN:HA	1.86	0.76
2:H:96:TRP:HZ3	3:I:24:LYS:HZ1	1.33	0.75
2:H:78:ASN:HB2	5:H:571:HOH:O	1.87	0.75
1:L:14(I):SER:HA	1:L:14(M):GLY:C	2.06	0.75
3:I:11:GLN:HA	3:I:45:THR:O	1.89	0.73
2:H:185:LYS:O	2:H:186(B):GLU:HB2	1.92	0.70
3:I:12:ASN:N	3:I:45:THR:O	2.24	0.70
3:I:29:ILE:HG12	3:I:40:VAL:CG1	2.21	0.70
3:I:58:GLU:HB3	5:I:722:HOH:O	1.90	0.69
2:H:174:ILE:HD11	3:I:21:VAL:CG2	2.21	0.69
2:H:195:SER:HB2	5:H:538:HOH:O	1.92	0.69
2:H:96:TRP:O	2:H:97(A):GLU:N	2.25	0.69
2:H:60(B):PRO:HG2	2:H:96:TRP:CZ2	2.28	0.69
3:I:31:GLY:HA3	3:I:36:GLY:O	1.92	0.68
3:I:12:ASN:O	3:I:46:PRO:HA	1.94	0.67
2:H:185:LYS:CB	2:H:186(B):GLU:HG3	2.19	0.67
3:I:27:LYS:CG	3:I:40:VAL:HG22	2.25	0.67
1:L:1(B):ALA:O	5:L:447:HOH:O	2.12	0.66
3:I:30:LEU:HA	3:I:37:ASN:ND2	2.11	0.66
2:H:230:HIS:HE1	2:H:232:PHE:HB3	1.61	0.66
2:H:46:LEU:HD22	2:H:48:SER:O	1.96	0.65
2:H:70:LYS:HE3	2:H:72:SER:O	1.97	0.64
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.32	0.64
3:I:30:LEU:HD23	3:I:37:ASN:ND2	2.13	0.64
2:H:164:GLU:HB2	2:H:166:PRO:HD2	1.80	0.62
1:L:1(C):GLU:HB2	5:L:447:HOH:O	2.00	0.62
2:H:35:ARG:NH1	2:H:35:ARG:HG3	2.10	0.62
2:H:17:VAL:O	2:H:18:GLU:HB2	1.99	0.61
3:I:53:ASN:ND2	5:I:574:HOH:O	2.34	0.61
3:I:29:ILE:HG12	3:I:40:VAL:HG11	1.81	0.61
2:H:85:LEU:HD13	2:H:106:MET:HG2	1.82	0.61
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.36	0.61
3:I:62:GLU:HB3	5:I:472:HOH:O	2.02	0.60
3:I:11:GLN:CA	3:I:45:THR:O	2.49	0.60
2:H:96:TRP:CH2	2:H:97:ARG:HG3	2.36	0.59
3:I:7:THR:HG22	3:I:8:GLU:HG3	1.84	0.59
2:H:35:ARG:CB	2:H:39:GLU:HG2	2.32	0.59
2:H:185:LYS:HG3	2:H:225:TYR:OH	2.03	0.58
2:H:124:PRO:O	2:H:235:LYS:HE2	2.04	0.58
2:H:51:TRP:CE2	2:H:242:ILE:HG12	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:LYS:HD2	2:H:89:TYR:CZ	2.39	0.57
2:H:60(D):TRP:CD2	3:I:49:GLU:HB2	2.39	0.57
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.53	0.57
3:I:60:PRO:HG2	3:I:63:TYR:HE2	1.70	0.57
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.40	0.56
2:H:51:TRP:CZ2	2:H:107:LYS:HD2	2.40	0.56
1:L:14(D):ARG:HG3	1:L:14(H):GLU:OE2	2.05	0.56
2:H:60(B):PRO:N	2:H:60(C):PRO:HD2	2.20	0.56
2:H:96:TRP:HZ3	3:I:24:LYS:NZ	2.03	0.56
2:H:77(A):ARG:HD2	5:I:467:HOH:O	2.04	0.56
2:H:94:TYR:HE1	2:H:99:LEU:HD12	1.71	0.55
3:I:65:GLN:HA	5:I:615:HOH:O	2.06	0.55
2:H:165:ARG:NH2	2:H:177:THR:O	2.38	0.55
2:H:17:VAL:O	2:H:188:GLY:HA2	2.06	0.55
1:L:14(A):LYS:NZ	5:L:684:HOH:O	2.35	0.55
2:H:66:VAL:HG21	2:H:106:MET:CE	2.37	0.54
3:I:27:LYS:N	3:I:40:VAL:O	2.39	0.54
2:H:49:ASP:O	2:H:111:PRO:HA	2.07	0.54
2:H:126:ARG:HG2	5:H:575:HOH:O	2.07	0.54
2:H:217:GLU:OE2	3:I:21:VAL:HG22	2.08	0.53
2:H:22:ALA:O	2:H:71:HIS:HE1	1.90	0.53
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.38	0.53
3:I:54:GLY:HA3	5:I:564:HOH:O	2.08	0.52
2:H:70:LYS:CE	2:H:72:SER:O	2.57	0.52
3:I:29:ILE:HG12	3:I:40:VAL:HG13	1.92	0.52
2:H:85:LEU:HD22	2:H:106:MET:HG2	1.93	0.51
3:I:60:PRO:HG2	3:I:63:TYR:CE2	2.44	0.51
2:H:192:GLU:HG3	5:H:414:HOH:O	2.09	0.51
2:H:60(B):PRO:N	2:H:60(C):PRO:CD	2.74	0.51
2:H:60(G):ASN:HB2	5:H:442:HOH:O	2.10	0.51
3:I:16:CYS:HB3	5:I:502:HOH:O	2.10	0.51
1:L:14(D):ARG:O	1:L:14(H):GLU:HG2	2.11	0.51
2:H:185:LYS:HD3	5:H:421:HOH:O	2.11	0.51
2:H:20:SER:O	2:H:156:GLN:HA	2.11	0.51
2:H:230:HIS:CE1	2:H:232:PHE:HB3	2.44	0.51
2:H:96:TRP:CZ3	2:H:97:ARG:HG3	2.46	0.50
2:H:101:ARG:NE	5:H:624:HOH:O	2.17	0.50
2:H:21:ASP:HB3	2:H:154:VAL:CG1	2.41	0.50
3:I:26:ASN:HA	3:I:40:VAL:O	2.11	0.50
3:I:3:TYR:HB3	3:I:15:LEU:HD13	1.93	0.50
2:H:130:LEU:HD23	2:H:162:ILE:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:52:ASN:C	3:I:53:ASN:HD22	2.16	0.49
2:H:164:GLU:HG3	5:H:694:HOH:O	2.13	0.49
3:I:61:GLU:HB3	5:I:451:HOH:O	2.13	0.48
2:H:203:SER:HB2	5:H:562:HOH:O	2.13	0.48
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	2.13	0.48
2:H:164:GLU:C	2:H:166:PRO:HD2	2.34	0.48
2:H:99:LEU:HD12	2:H:99:LEU:HA	1.80	0.48
2:H:70:LYS:NZ	2:H:75:ARG:O	2.47	0.48
3:I:61:GLU:HA	3:I:64:LEU:HB2	1.95	0.48
2:H:60:LEU:CD1	4:H:400:NAG:H5	2.44	0.48
2:H:46:LEU:CD2	2:H:48:SER:O	2.62	0.47
3:I:65:GLN:HG3	5:I:615:HOH:O	2.14	0.47
1:L:5:PRO:O	1:L:10:LYS:HG3	2.14	0.47
2:H:35:ARG:NH1	2:H:39:GLU:OE2	2.47	0.47
2:H:239:GLN:NE2	5:H:689:HOH:O	2.46	0.47
2:H:98:ASN:HA	2:H:98:ASN:HD22	1.35	0.47
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.14	0.47
2:H:56:ALA:N	2:H:102:ASP:OD1	2.47	0.47
1:L:5:PRO:HA	1:L:9:LYS:HB2	1.96	0.47
2:H:91:HIS:CE1	2:H:101:ARG:CD	2.94	0.47
2:H:94:TYR:CE1	2:H:99:LEU:HD12	2.49	0.47
2:H:204(B):ASN:ND2	2:H:206:ARG:HB2	2.30	0.47
2:H:192:GLU:HG2	3:I:2:THR:HB	1.98	0.46
1:L:9:LYS:HE2	5:L:614:HOH:O	2.16	0.46
2:H:60:LEU:HD13	4:H:400:NAG:H5	1.97	0.46
2:H:33:LEU:HD21	2:H:106:MET:CE	2.46	0.46
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.18	0.46
2:H:99:LEU:O	2:H:102:ASP:HB2	2.16	0.46
2:H:85:LEU:CD1	2:H:106:MET:HG2	2.46	0.45
3:I:59:ILE:HD11	3:I:64:LEU:HD13	1.98	0.45
2:H:79:ILE:HD12	5:H:593:HOH:O	2.16	0.45
2:H:73:ARG:HB2	2:H:141:TRP:HD1	1.78	0.45
1:L:1(A):ASP:OD1	1:L:3:LEU:HD12	2.17	0.45
2:H:41:LEU:CD1	2:H:64:LEU:HD23	2.48	0.44
2:H:236:LYS:HD3	2:H:236:LYS:HA	1.77	0.44
5:H:713:HOH:O	3:I:24:LYS:HE2	2.16	0.44
2:H:169:LYS:HE2	2:H:169:LYS:HB3	1.65	0.44
2:H:69:GLY:HA2	2:H:117:TYR:O	2.18	0.44
2:H:66:VAL:CG2	2:H:106:MET:CE	2.95	0.43
2:H:136:GLY:O	2:H:160:LEU:N	2.44	0.43
2:H:160:LEU:HA	2:H:161:PRO:HD3	1.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:ILE:HG22	2:H:91:HIS:O	2.19	0.43
2:H:29:TRP:O	2:H:45:SER:HA	2.18	0.43
3:I:27:LYS:O	3:I:40:VAL:N	2.42	0.43
1:L:14(F):LEU:HD12	2:H:207:TRP:CH2	2.53	0.43
3:I:3:TYR:CB	3:I:15:LEU:HD13	2.49	0.43
3:I:30:LEU:CD2	3:I:37:ASN:HD21	2.32	0.43
3:I:54:GLY:N	3:I:55:ASP:OD1	2.52	0.43
2:H:80:GLU:O	5:H:583:HOH:O	2.21	0.43
2:H:41:LEU:HD12	2:H:64:LEU:HD23	2.01	0.42
3:I:7:THR:N	3:I:11:GLN:OE1	2.48	0.42
3:I:52:ASN:N	5:I:574:HOH:O	2.51	0.42
2:H:165:ARG:N	2:H:166:PRO:CD	2.83	0.42
2:H:77(A):ARG:CD	5:I:467:HOH:O	2.64	0.42
2:H:57:HIS:CD2	3:I:1:ILE:HG12	2.55	0.42
3:I:52:ASN:C	3:I:53:ASN:ND2	2.73	0.42
2:H:105:LEU:HD13	2:H:241:VAL:HG22	2.01	0.42
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.85	0.42
3:I:7:THR:CG2	3:I:8:GLU:HG3	2.48	0.42
1:L:14:ASP:OD2	1:L:14(C):GLU:HG3	2.20	0.42
2:H:50:ARG:HD3	2:H:107:LYS:HE2	2.01	0.42
2:H:144:LEU:HA	2:H:144:LEU:HD23	1.74	0.42
3:I:45:THR:HG23	3:I:46:PRO:HD2	2.01	0.42
1:L:14:ASP:CG	1:L:14(C):GLU:HG3	2.41	0.42
3:I:52:ASN:HB3	5:I:569:HOH:O	2.19	0.41
2:H:85:LEU:CD2	2:H:106:MET:HG2	2.51	0.41
2:H:182:CYS:HA	2:H:226:GLY:O	2.20	0.41
2:H:51:TRP:CD2	2:H:242:ILE:HG12	2.55	0.41
1:L:14(H):GLU:H	1:L:14(H):GLU:HG2	1.39	0.41
1:L:14(D):ARG:CG	1:L:14(H):GLU:OE2	2.68	0.41
1:L:14(F):LEU:HD12	2:H:207:TRP:HH2	1.84	0.41
2:H:228:TYR:N	2:H:228:TYR:CD1	2.89	0.41
3:I:26:ASN:CA	3:I:40:VAL:O	2.69	0.41
2:H:103:ILE:CD1	5:H:529:HOH:O	2.68	0.41
2:H:165:ARG:N	2:H:166:PRO:HD2	2.35	0.41
2:H:234:LEU:HB2	5:H:529:HOH:O	2.20	0.41
3:I:63:TYR:HE2	5:I:657:HOH:O	2.03	0.41
2:H:184(A):TYR:CZ	2:H:186(D):LYS:HD3	2.56	0.41
2:H:187:ARG:HD2	2:H:187:ARG:HH11	1.53	0.41
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.19	0.40
2:H:221(A):ARG:HB2	5:H:580:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(E):SER:O	2:H:146:GLU:O[5_645]	2.13	0.07

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%)	7 (23%)	0	100 100
2	H	256/259 (99%)	241 (94%)	12 (5%)	3 (1%)	13 14
3	I	57/65 (88%)	51 (90%)	5 (9%)	1 (2%)	8 7
All	All	344/360 (96%)	316 (92%)	24 (7%)	4 (1%)	13 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97	ARG
2	H	97(A)	GLU
2	H	98	ASN
3	I	53	ASN

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	26/31 (84%)	20 (77%)	6 (23%)	1 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	222/225 (99%)	198 (89%)	24 (11%)	6 7
3	I	51/55 (93%)	41 (80%)	10 (20%)	1 1
All	All	299/311 (96%)	259 (87%)	40 (13%)	4 4

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	6	LEU
1	L	9	LYS
1	L	14(D)	ARG
1	L	14(G)	LEU
1	L	14(H)	GLU
2	H	35	ARG
2	H	46	LEU
2	H	50	ARG
2	H	61	GLU
2	H	64	LEU
2	H	87	LYS
2	H	93	ARG
2	H	98	ASN
2	H	99	LEU
2	H	106	MET
2	H	112	VAL
2	H	127	GLU
2	H	129(B)	SER
2	H	147	THR
2	H	151	GLN
2	H	176	ILE
2	H	182	CYS
2	H	185	LYS
2	H	187	ARG
2	H	195	SER
2	H	204(B)	ASN
2	H	233	ARG
2	H	234	LEU
2	H	245	PHE
3	I	7	THR
3	I	21	VAL
3	I	29	ILE
3	I	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	40	VAL
3	I	53	ASN
3	I	55	ASP
3	I	58	GLU
3	I	64	LEU
3	I	65	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	71	HIS
2	H	98	ASN
2	H	204(B)	ASN
2	H	239	GLN
3	I	37	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\|>2$
4	NAG	H	400	2	14,14,15	0.42	0	17,19,21	0.76	1 (5%)

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
4	NAG	H	400	2	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	400	NAG	C1-O5-C5	2.03	114.94	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	400	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	400	NAG	C8-C7-N2-C2
4	H	400	NAG	O7-C7-N2-C2
4	H	400	NAG	C4-C5-C6-O6
4	H	400	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	400	NAG	2	0

5.7 Other polymers (i)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.