Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:20 PM GMT

PDB ID	:	1ABI
Title	:	STRUCTURE OF THE HIRULOG 3-THROMBIN COMPLEX AND NATURE OF THE S' SUBSITES OF SUBSTRATES AND INHIBITORS
Authors	:	Qiu, X.; Tulinsky, A.
Deposited on	:	1992-08-24
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
http://wwpdb.org/validation/2016/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:

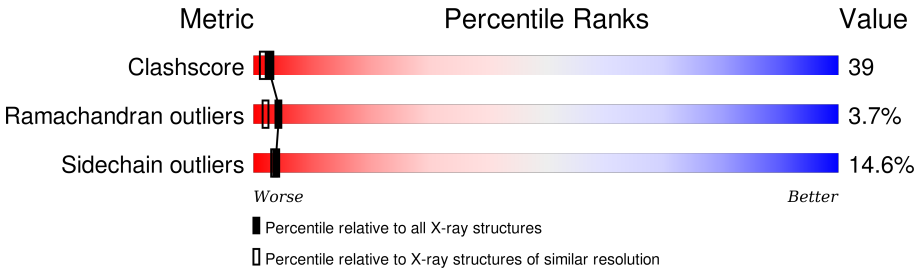
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	19% 36% 22% 14% 8%
2	H	259	42% 39% 13%
3	I	20	15% 40% 30% 15%

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
3	DPN	I	56	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2703 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
			265	162	45	57	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2039	1299	360	366	14			

- Molecule 3 is a protein called HIRULOG 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	20	Total	C	N	O	0	0	0
			153	96	24	33			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	199	Total	O	0	0
			199	199		
4	I	18	Total	O	0	0
			18	18		
4	L	29	Total	O	0	0
			29	29		

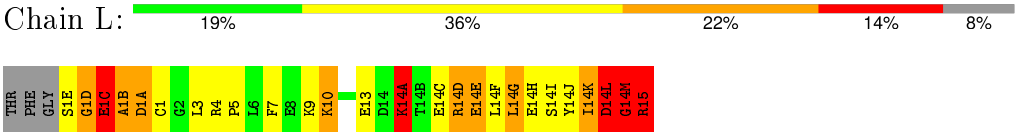
3 Residue-property plots (i)

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.

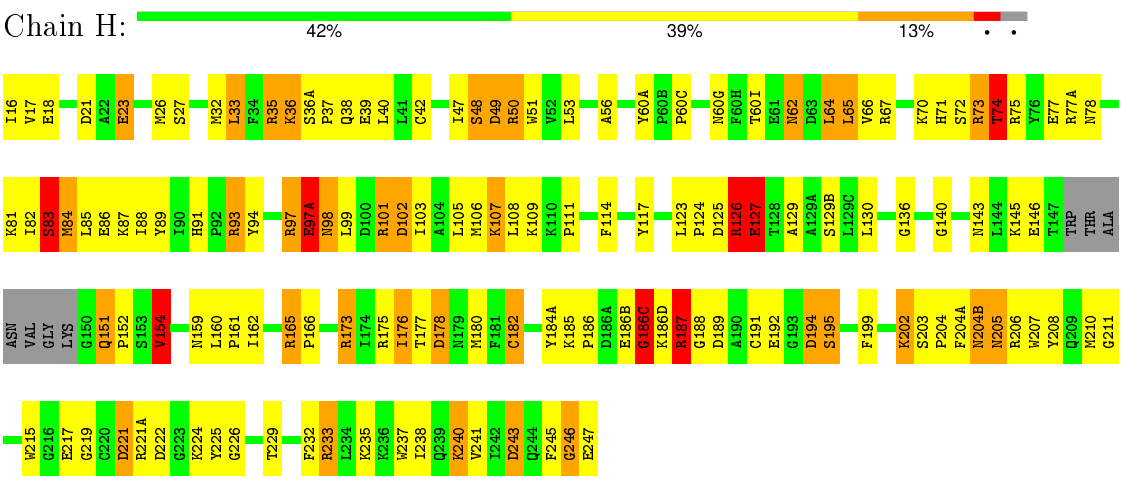
- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L:



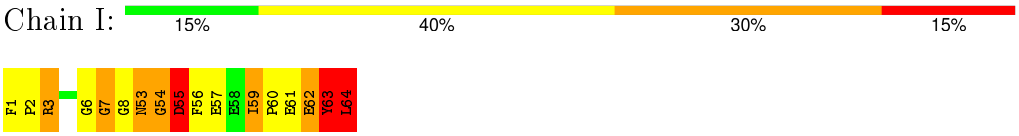
- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H:



- Molecule 3: HIRULOG 3

Chain I:



4 Data and refinement statistics (i)

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	71.44Å 72.10Å 73.07Å 90.00° 101.02° 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	PROLSQ	Depositor
R, R_{free}	0.132 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2703	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: DPN, HMR

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	1.10	0/267	2.52	19/353 (5.4%)
2	H	1.11	2/2091 (0.1%)	2.32	82/2823 (2.9%)
3	I	1.13	0/119	1.94	4/154 (2.6%)
All	All	1.11	2/2477 (0.1%)	2.33	105/3330 (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
3	I	1	2
All	All	1	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	219	GLY	N-CA	6.21	1.55	1.46
2	H	77(A)	ARG	C-O	5.76	1.34	1.23

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	187	ARG	NE-CZ-NH1	20.58	130.59	120.30
2	H	187	ARG	NE-CZ-NH2	-18.23	111.18	120.30
2	H	101	ARG	NE-CZ-NH1	18.21	129.41	120.30
2	H	101	ARG	NE-CZ-NH2	-18.02	111.29	120.30
2	H	73	ARG	NE-CZ-NH1	16.52	128.56	120.30
2	H	233	ARG	NE-CZ-NH2	-15.72	112.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	35	ARG	NE-CZ-NH2	-13.81	113.39	120.30
2	H	73	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	L	15	ARG	CD-NE-CZ	13.14	142.00	123.60
2	H	93	ARG	NE-CZ-NH1	12.54	126.57	120.30
2	H	67	ARG	NE-CZ-NH1	12.50	126.55	120.30
2	H	93	ARG	CD-NE-CZ	11.33	139.46	123.60
1	L	14(D)	ARG	CD-NE-CZ	11.26	139.37	123.60
1	L	14(D)	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	L	1(A)	ASP	CB-CG-OD1	-10.93	108.47	118.30
2	H	221(A)	ARG	NE-CZ-NH2	10.41	125.51	120.30
2	H	33	LEU	CA-CB-CG	10.35	139.10	115.30
2	H	175	ARG	NE-CZ-NH1	10.34	125.47	120.30
2	H	21	ASP	CB-CG-OD1	10.14	127.43	118.30
2	H	165	ARG	NE-CZ-NH2	9.94	125.27	120.30
2	H	75	ARG	NE-CZ-NH1	9.59	125.09	120.30
2	H	35	ARG	NE-CZ-NH1	9.41	125.01	120.30
2	H	125	ASP	CB-CG-OD1	9.40	126.76	118.30
2	H	178	ASP	CB-CG-OD2	-9.40	109.84	118.30
2	H	126	ARG	NE-CZ-NH2	-9.38	115.61	120.30
2	H	221	ASP	CB-CG-OD2	8.61	126.05	118.30
1	L	1(A)	ASP	CB-CA-C	8.54	127.48	110.40
2	H	117	TYR	CB-CG-CD2	-8.54	115.88	121.00
2	H	83	SER	N-CA-CB	8.53	123.30	110.50
2	H	32	MET	CG-SD-CE	8.41	113.66	100.20
2	H	93	ARG	NE-CZ-NH2	-8.31	116.14	120.30
2	H	225	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	L	14(K)	ILE	CB-CA-C	8.01	127.62	111.60
2	H	97	ARG	CD-NE-CZ	-8.01	112.38	123.60
2	H	173	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	H	243	ASP	CB-CG-OD1	7.86	125.37	118.30
2	H	126	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	H	206	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	H	233	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	L	13	GLU	CA-CB-CG	7.75	130.44	113.40
2	H	49	ASP	CB-CG-OD1	-7.63	111.44	118.30
2	H	125	ASP	CB-CG-OD2	-7.55	111.50	118.30
2	H	189	ASP	CB-CG-OD1	-7.54	111.52	118.30
2	H	102	ASP	CB-CG-OD1	-7.31	111.72	118.30
2	H	77	GLU	OE1-CD-OE2	-7.25	114.60	123.30
2	H	127	GLU	CB-CG-CD	7.17	133.56	114.20
1	L	14(C)	GLU	CG-CD-OE1	-7.04	104.21	118.30
2	H	67	ARG	NH1-CZ-NH2	-6.46	112.29	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	186(D)	LYS	N-CA-C	-6.45	93.59	111.00
3	I	63	TYR	C-N-CA	6.43	137.78	121.70
2	H	165	ARG	CD-NE-CZ	-6.40	114.64	123.60
2	H	97	ARG	NE-CZ-NH1	-6.21	117.19	120.30
2	H	186(D)	LYS	N-CA-CB	6.21	121.77	110.60
2	H	114	PHE	CB-CG-CD1	-6.15	116.50	120.80
2	H	94	TYR	CB-CG-CD2	-6.13	117.33	121.00
2	H	74	THR	CA-CB-OG1	-6.12	96.14	109.00
2	H	94	TYR	CB-CG-CD1	6.12	124.67	121.00
2	H	140	GLY	CA-C-O	6.11	131.60	120.60
2	H	114	PHE	O-C-N	6.08	132.42	122.70
2	H	78	ASN	CA-CB-CG	6.07	126.76	113.40
2	H	186(C)	GLY	C-N-CA	6.07	136.88	121.70
2	H	129(B)	SER	N-CA-CB	5.99	119.49	110.50
2	H	27	SER	N-CA-CB	-5.93	101.60	110.50
2	H	173	ARG	CG-CD-NE	5.91	124.21	111.80
1	L	1(A)	ASP	CB-CG-OD2	5.90	123.61	118.30
2	H	175	ARG	C-N-CA	5.89	136.43	121.70
2	H	83	SER	CA-C-N	-5.88	104.26	117.20
2	H	77(A)	ARG	C-N-CA	-5.83	107.13	121.70
2	H	208	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	H	154	VAL	N-CA-CB	-5.77	98.80	111.50
2	H	184(A)	TYR	CB-CG-CD1	-5.76	117.54	121.00
2	H	176	ILE	CA-CB-CG2	5.75	122.40	110.90
1	L	14(K)	ILE	CA-C-O	5.75	132.16	120.10
2	H	27	SER	CB-CA-C	5.72	120.96	110.10
1	L	14(M)	GLY	N-CA-C	5.71	127.37	113.10
2	H	21	ASP	CB-CG-OD2	-5.71	113.16	118.30
2	H	194	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	H	23	GLU	OE1-CD-OE2	5.68	130.12	123.30
2	H	117	TYR	CB-CG-CD1	5.60	124.36	121.00
1	L	14(E)	GLU	CB-CG-CD	5.59	129.31	114.20
2	H	62	ASN	CB-CA-C	-5.52	99.35	110.40
1	L	14(A)	LYS	N-CA-CB	5.47	120.44	110.60
2	H	97(A)	GLU	CA-CB-CG	5.46	125.42	113.40
2	H	173	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
2	H	127	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	L	1(B)	ALA	CA-C-O	5.33	131.29	120.10
2	H	74	THR	OG1-CB-CG2	5.32	122.24	110.00
2	H	246	GLY	O-C-N	5.30	131.19	122.70
2	H	127	GLU	CA-CB-CG	5.29	125.03	113.40
1	L	7	PHE	CB-CG-CD1	-5.28	117.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	74	THR	N-CA-C	5.25	125.17	111.00
2	H	97(A)	GLU	CA-C-N	5.23	128.70	117.20
3	I	64	LEU	N-CA-CB	-5.20	100.00	110.40
2	H	217	GLU	OE1-CD-OE2	-5.17	117.09	123.30
2	H	66	VAL	CA-CB-CG1	5.16	118.64	110.90
3	I	57	GLU	OE1-CD-OE2	5.16	129.49	123.30
2	H	49	ASP	CB-CG-OD2	5.12	122.91	118.30
1	L	14(D)	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	I	57	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	L	14(G)	LEU	CB-CA-C	5.08	119.86	110.20
2	H	98	ASN	N-CA-CB	-5.06	101.48	110.60
1	L	4	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	L	10	LYS	CB-CA-C	-5.03	100.33	110.40
2	H	56	ALA	N-CA-CB	5.01	117.11	110.10
2	H	77	GLU	CA-C-O	5.01	130.61	120.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	56	DPN	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	187	ARG	Sidechain
3	I	3	HMR	Mainchain,Peptide

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	265	0	259	42	2
2	H	2039	0	2010	145	1
3	I	153	0	128	34	0
4	H	199	0	0	18	0
4	I	18	0	0	4	0
4	L	29	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2703	0	2397	191	2

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 39.

All (191) 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)
2:H:205:ASN:HB3	4:H:593:HOH:O	1.36	1.22
3:I:61:GLU:CD	4:I:572:HOH:O	1.83	1.15
2:H:224:LYS:HE2	4:H:585:HOH:O	1.48	1.12
1:L:1(E):SER:HB2	2:H:123:LEU:O	1.49	1.12
2:H:240:LYS:HZ2	2:H:240:LYS:HB3	0.97	1.11
2:H:82:ILE:HD12	3:I:63:TYR:CD2	1.87	1.09
2:H:240:LYS:NZ	2:H:240:LYS:HB3	1.65	1.06
1:L:9:LYS:CD	4:L:526:HOH:O	2.04	1.05
1:L:10:LYS:HE3	4:L:501:HOH:O	1.53	1.04
1:L:15:ARG:HB2	2:H:204:PRO:O	1.57	1.03
1:L:9:LYS:HD2	4:L:526:HOH:O	1.56	1.02
2:H:36:LYS:HG3	2:H:65:LEU:HD22	1.41	1.01
2:H:50:ARG:HH11	2:H:107:LYS:HE2	1.26	0.99
2:H:73:ARG:HD3	2:H:152:PRO:O	1.61	0.97
2:H:50:ARG:NH1	2:H:107:LYS:HE2	1.80	0.97
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.67	0.93
1:L:15:ARG:NH1	2:H:204(A):PHE:O	2.00	0.93
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.50	0.90
2:H:240:LYS:CB	2:H:240:LYS:HZ2	1.81	0.89
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.55	0.88
1:L:10:LYS:CE	4:L:501:HOH:O	2.15	0.86
3:I:53:ASN:O	3:I:55:ASP:N	2.08	0.86
2:H:85:LEU:HD13	2:H:106:MET:CE	2.07	0.83
2:H:17:VAL:O	2:H:188:GLY:HA2	1.78	0.83
2:H:82:ILE:HD12	3:I:63:TYR:HD2	1.38	0.82
2:H:240:LYS:CB	2:H:240:LYS:NZ	2.29	0.80
2:H:187:ARG:NH1	2:H:221:ASP:O	2.16	0.79
2:H:146:GLU:HB2	4:H:624:HOH:O	1.81	0.79
1:L:1(E):SER:CB	2:H:123:LEU:O	2.30	0.78
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.17	0.78
2:H:40:LEU:O	3:I:6:GLY:O	2.04	0.76
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.86	0.75
2:H:195:SER:HB3	3:I:3:HMR:HC1	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:LEU:HD11	2:H:84:MET:CE	2.16	0.75
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	1.87	0.74
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.87	0.74
1:L:14(J):TYR:C	1:L:14(K):ILE:HG13	2.06	0.73
2:H:50:ARG:NH1	2:H:107:LYS:CE	2.51	0.73
3:I:61:GLU:CG	4:I:572:HOH:O	2.31	0.72
2:H:129:ALA:O	2:H:130:LEU:HB2	1.89	0.71
2:H:178:ASP:O	2:H:233:ARG:HD2	1.91	0.70
2:H:146:GLU:N	4:H:624:HOH:O	2.00	0.70
3:I:54:GLY:O	3:I:56:DPN:N	2.25	0.70
2:H:224:LYS:CE	4:H:585:HOH:O	2.19	0.69
3:I:53:ASN:C	3:I:55:ASP:H	1.96	0.69
3:I:64:LEU:OXT	3:I:64:LEU:HD13	1.93	0.69
1:L:1(D):GLY:H	2:H:123:LEU:H	1.42	0.68
2:H:143:ASN:ND2	2:H:192:GLU:HG2	2.07	0.68
2:H:109:LYS:HE3	4:H:623:HOH:O	1.92	0.68
2:H:35:ARG:O	2:H:38:GLN:HA	1.96	0.66
1:L:15:ARG:NH1	4:L:469:HOH:O	2.28	0.65
2:H:99:LEU:HD21	3:I:2:PRO:HB3	1.77	0.65
2:H:187:ARG:HH22	2:H:222:ASP:CG	1.99	0.65
2:H:105:LEU:HD12	2:H:241:VAL:CG2	2.27	0.65
1:L:1(C):GLU:OE2	4:L:618:HOH:O	2.15	0.64
1:L:14(A):LYS:HD3	2:H:23:GLU:CD	2.18	0.64
1:L:10:LYS:NZ	4:L:560:HOH:O	2.22	0.63
3:I:64:LEU:OXT	3:I:64:LEU:CD1	2.47	0.63
1:L:15:ARG:HD2	2:H:204:PRO:O	1.99	0.63
1:L:14(A):LYS:HD3	2:H:23:GLU:OE1	1.98	0.63
2:H:65:LEU:HD11	2:H:84:MET:HE1	1.79	0.63
2:H:237:TRP:O	2:H:241:VAL:HG13	1.99	0.63
1:L:14(J):TYR:C	1:L:14(K):ILE:CG1	2.67	0.62
2:H:85:LEU:CD1	2:H:106:MET:CE	2.78	0.62
2:H:60(I):THR:CB	2:H:62:ASN:HD22	2.13	0.62
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.81	0.61
2:H:182:CYS:HA	2:H:226:GLY:O	2.00	0.61
2:H:65:LEU:HD11	2:H:84:MET:HE2	1.82	0.60
2:H:36:LYS:CG	2:H:65:LEU:HD22	2.26	0.60
2:H:105:LEU:HD12	2:H:241:VAL:HG22	1.82	0.60
2:H:124:PRO:O	2:H:235:LYS:NZ	2.35	0.60
3:I:59:ILE:HD11	3:I:64:LEU:CD2	2.32	0.60
1:L:1(D):GLY:HA3	2:H:123:LEU:H	1.67	0.60
2:H:82:ILE:CD1	3:I:63:TYR:CD2	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:ARG:NH1	4:H:482:HOH:O	2.36	0.58
1:L:1(E):SER:O	1:L:1(C):GLU:N	2.28	0.58
2:H:36:LYS:HE3	4:H:534:HOH:O	2.04	0.57
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.34	0.57
2:H:91:HIS:CE1	2:H:93:ARG:HB2	2.38	0.57
3:I:59:ILE:HB	3:I:60:PRO:HD2	1.86	0.57
3:I:61:GLU:HG2	4:I:572:HOH:O	2.00	0.57
2:H:50:ARG:NH1	2:H:108:LEU:O	2.38	0.57
2:H:39:GLU:HB2	3:I:8:GLY:HA2	1.86	0.56
2:H:126:ARG:CB	2:H:126:ARG:HH11	2.18	0.56
1:L:1(D):GLY:N	2:H:123:LEU:H	2.02	0.56
1:L:15:ARG:HD3	4:L:591:HOH:O	2.05	0.56
2:H:185:LYS:HB2	2:H:186(B):GLU:CG	2.31	0.56
2:H:130:LEU:HG	2:H:210:MET:HE3	1.88	0.56
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.70	0.56
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.41	0.56
3:I:53:ASN:C	3:I:55:ASP:N	2.57	0.55
2:H:195:SER:CB	3:I:3:HMR:HC1	2.36	0.55
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.41	0.55
1:L:1(D):GLY:O	1:L:1(C):GLU:HB2	2.07	0.55
1:L:1(D):GLY:CA	2:H:123:LEU:H	2.21	0.54
2:H:36(A):SER:HA	2:H:37:PRO:C	2.28	0.54
1:L:5:PRO:HA	1:L:9:LYS:CG	2.38	0.53
2:H:87:LYS:HD2	2:H:88:ILE:H	1.72	0.53
1:L:10:LYS:NZ	4:L:620:HOH:O	2.29	0.53
1:L:1(C):GLU:CB	1:L:1:CYS:HB3	2.39	0.53
3:I:62:GLU:CD	4:I:568:HOH:O	2.47	0.53
2:H:35:ARG:HB3	2:H:37:PRO:O	2.09	0.52
1:L:15:ARG:CZ	4:L:469:HOH:O	2.58	0.52
3:I:59:ILE:HD11	3:I:64:LEU:HD23	1.92	0.52
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.25	0.51
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.45	0.51
2:H:165:ARG:NH1	4:H:613:HOH:O	2.25	0.51
2:H:202:LYS:HG3	2:H:207:TRP:CE2	2.45	0.51
2:H:50:ARG:CD	2:H:108:LEU:O	2.59	0.51
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.92	0.51
2:H:73:ARG:NE	2:H:151:GLN:HB2	2.26	0.51
2:H:165:ARG:N	2:H:166:PRO:HD2	2.26	0.51
2:H:60(I):THR:HB	2:H:62:ASN:ND2	2.25	0.51
2:H:82:ILE:HD12	3:I:63:TYR:CE2	2.42	0.50
2:H:87:LYS:HG3	2:H:89:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:SER:HB3	4:H:445:HOH:O	2.12	0.50
2:H:60(C):PRO:HB2	4:H:464:HOH:O	2.11	0.50
1:L:1(C):GLU:HB3	1:L:1:CYS:HB3	1.95	0.49
2:H:211:GLY:HA2	2:H:229:THR:O	2.11	0.49
2:H:205:ASN:CB	4:H:593:HOH:O	2.18	0.49
2:H:126:ARG:HB3	2:H:126:ARG:HH11	1.77	0.49
2:H:51:TRP:CZ3	2:H:107:LYS:HB3	2.48	0.48
2:H:235:LYS:O	2:H:238:ILE:HB	2.14	0.48
2:H:70:LYS:HE3	2:H:72:SER:O	2.14	0.48
2:H:60(I):THR:HB	2:H:62:ASN:HD22	1.79	0.48
2:H:105:LEU:HD12	2:H:241:VAL:HG21	1.96	0.47
2:H:99:LEU:O	2:H:102:ASP:HB2	2.14	0.47
2:H:42:CYS:HB3	2:H:195:SER:O	2.14	0.47
2:H:16:ILE:N	2:H:194:ASP:OD2	2.47	0.47
2:H:97(A):GLU:HB2	4:H:599:HOH:O	2.15	0.47
1:L:14(E):GLU:HB2	4:L:434:HOH:O	2.14	0.47
2:H:48:SER:OG	2:H:49:ASP:N	2.47	0.47
2:H:74:THR:OG1	3:I:56:DPN:HA	2.15	0.47
2:H:39:GLU:HB2	3:I:7:GLY:O	2.14	0.47
2:H:88:ILE:HG21	2:H:88:ILE:HD13	1.73	0.47
2:H:39:GLU:OE1	3:I:8:GLY:HA2	2.14	0.46
2:H:203:SER:O	2:H:205:ASN:HA	2.16	0.46
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.51	0.46
1:L:1(D):GLY:HA3	2:H:123:LEU:N	2.30	0.46
3:I:61:GLU:O	3:I:62:GLU:O	2.33	0.46
2:H:146:GLU:CB	4:H:624:HOH:O	2.47	0.46
2:H:165:ARG:NH2	2:H:180:MET:O	2.49	0.46
2:H:60(G):ASN:ND2	4:H:436:HOH:O	2.27	0.46
2:H:126:ARG:HA	2:H:232:PHE:CZ	2.52	0.45
2:H:73:ARG:CZ	2:H:151:GLN:HB2	2.46	0.45
2:H:107:LYS:HB2	2:H:107:LYS:HE3	1.48	0.45
3:I:59:ILE:CG1	3:I:64:LEU:HD23	2.47	0.45
2:H:215:TRP:HB2	3:I:1:DPN:O	2.17	0.45
2:H:176:ILE:HD13	2:H:176:ILE:N	2.31	0.45
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.20	0.44
1:L:14(D):ARG:HE	1:L:14(H):GLU:CD	2.21	0.44
2:H:17:VAL:O	2:H:18:GLU:HB2	2.18	0.44
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.50	0.44
2:H:126:ARG:NH1	2:H:126:ARG:CG	2.78	0.44
2:H:224:LYS:O	4:H:421:HOH:O	2.21	0.44
2:H:152:PRO:HB2	2:H:154:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:LYS:HB2	4:H:592:HOH:O	2.17	0.44
2:H:97:ARG:HD2	2:H:97:ARG:HH11	1.40	0.43
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.19	0.43
2:H:136:GLY:O	2:H:159:ASN:HA	2.18	0.43
2:H:50:ARG:HD3	2:H:108:LEU:O	2.19	0.43
3:I:62:GLU:O	3:I:64:LEU:N	2.52	0.43
1:L:15:ARG:HG2	4:L:591:HOH:O	2.18	0.43
1:L:9:LYS:CE	4:L:526:HOH:O	2.58	0.43
2:H:107:LYS:NZ	2:H:246:GLY:HA2	2.34	0.43
2:H:191:CYS:O	2:H:194:ASP:HB2	2.18	0.43
2:H:151:GLN:HG2	2:H:151:GLN:H	1.49	0.43
2:H:143:ASN:ND2	2:H:192:GLU:CG	2.79	0.43
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.54	0.43
2:H:186:PRO:HD3	4:H:449:HOH:O	2.18	0.42
2:H:64:LEU:HD12	2:H:85:LEU:HD12	2.00	0.42
2:H:82:ILE:HG13	3:I:63:TYR:CE2	2.53	0.42
1:L:14(G):LEU:HD22	1:L:14(G):LEU:N	2.34	0.42
2:H:186(B):GLU:O	2:H:186(C):GLY:C	2.57	0.42
2:H:232:PHE:O	2:H:235:LYS:HB2	2.19	0.42
3:I:54:GLY:C	3:I:56:DPN:N	2.73	0.42
2:H:129:ALA:HA	2:H:210:MET:HE1	2.02	0.42
2:H:98:ASN:HD21	2:H:177:THR:CG2	2.33	0.41
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.54	0.41
1:L:3:LEU:O	1:L:9:LYS:HE3	2.21	0.41
2:H:126:ARG:HB3	2:H:127:GLU:OE1	2.21	0.41
2:H:87:LYS:HE3	2:H:88:ILE:O	2.21	0.41
1:L:3:LEU:HA	1:L:3:LEU:HD23	1.72	0.41
2:H:127:GLU:H	2:H:127:GLU:CD	2.25	0.41
2:H:160:LEU:HA	2:H:161:PRO:HD3	1.90	0.41
2:H:38:GLN:HE22	3:I:64:LEU:HD21	1.86	0.40
3:I:61:GLU:O	3:I:62:GLU:C	2.59	0.40
2:H:49:ASP:OD2	2:H:111:PRO:HB3	2.21	0.40
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.50	0.40
2:H:98:ASN:HA	3:I:1:DPN:HZ	2.02	0.40
4:L:549:HOH:O	2:H:26:MET:CE	2.69	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(M):GLY:O	2:H:173:ARG:NE[4_556]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14(H):GLU:OE2	1:L:14(L):ASP:OD2[2_556]	2.18	0.02

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%)	22 (71%)	4 (13%)	5 (16%)	0 0
2	H	248/259 (96%)	227 (92%)	20 (8%)	1 (0%)	39 48
3	I	16/20 (80%)	10 (62%)	1 (6%)	5 (31%)	0 0
All	All	295/315 (94%)	259 (88%)	25 (8%)	11 (4%)	4 2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(D)	GLY
1	L	1(C)	GLU
1	L	14(M)	GLY
3	I	54	GLY
3	I	55	ASP
3	I	63	TYR
1	L	14(L)	ASP
3	I	62	GLU
3	I	7	GLY
1	L	1(B)	ALA
2	H	186(C)	GLY

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%)	23 (79%)	6 (21%)	1 1
2	H	220/225 (98%)	193 (88%)	27 (12%)	6 6
3	I	11/11 (100%)	6 (54%)	5 (46%)	0 0
All	All	260/267 (97%)	222 (85%)	38 (15%)	4 3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	1(A)	ASP
1	L	14(A)	LYS
1	L	14(F)	LEU
1	L	14(L)	ASP
1	L	15	ARG
2	H	33	LEU
2	H	36	LYS
2	H	47	ILE
2	H	48	SER
2	H	50	ARG
2	H	64	LEU
2	H	65	LEU
2	H	74	THR
2	H	81	LYS
2	H	83	SER
2	H	84	MET
2	H	97(A)	GLU
2	H	107	LYS
2	H	126	ARG
2	H	127	GLU
2	H	145	LYS
2	H	151	GLN
2	H	154	VAL
2	H	182	CYS
2	H	195	SER
2	H	202	LYS
2	H	204(B)	ASN
2	H	205	ASN
2	H	240	LYS
2	H	243	ASP

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Mol	Chain	Res	Type
2	H	245	PHE
2	H	247	GLU
3	I	53	ASN
3	I	55	ASP
3	I	59	ILE
3	I	63	TYR
3	I	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	62	ASN
2	H	78	ASN
2	H	204(B)	ASN
2	H	205	ASN
2	H	244	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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	-	10,11,12	0.95	0	10,13,15	1.68	3 (30%)
3	HMR	I	3	3	8,11,12	0.76	0	7,12,14	2.89	2 (28%)
3	DPN	I	56	3	10,11,12	0.80	0	10,13,15	0.38	0

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	-	-	0/4/6/8	0/1/1/1
3	HMR	I	3	3	-	0/8/10/11	0/0/0/0
3	DPN	I	56	3	1/1/1/2	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3	HMR	CA-CH2-C	-7.05	101.13	112.32
3	I	1	DPN	O-C-CA	-2.83	118.13	125.49
3	I	3	HMR	O-C-CH2	-2.23	117.09	125.24
3	I	1	DPN	CE2-CD2-CG	-2.11	117.29	120.65
3	I	1	DPN	CG-CB-CA	3.07	121.15	114.21

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	56	DPN	CA

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	DPN	2	0
3	I	3	HMR	2	0
3	I	56	DPN	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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.