Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:24 PM GMT

PDB ID	:	1THR
Title	:	STRUCTURES OF THROMBIN COMPLEXES WITH A DESIGNED AND A NATURAL EXOSITE INHIBITOR
Authors	:	Qiu, X.; Yin, M.; Padmanabhan, K.P.; Krstenansky, J.L.; Tulinsky, A.
Deposited on	:	1993-06-16
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:

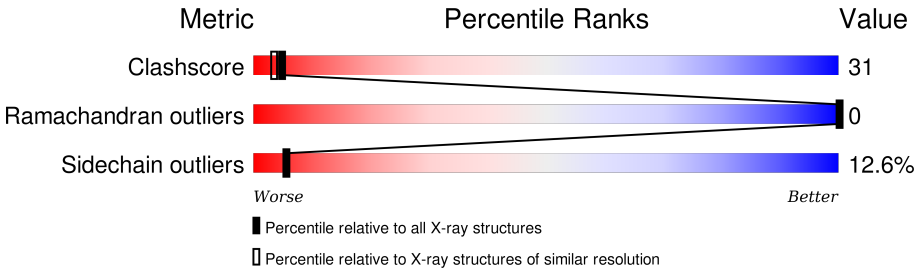
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	36% 31% 8% 25%
2	H	259	42% 36% 15% 5% •
3	I	13	15% 62% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2541 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	27	Total	C	N	O	S	0	0	1
			209	131	33	44	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
			2031	1295	359	363	14			

- Molecule 3 is a protein called HIRULLIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	0	0	0
			111	68	14	29			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	160	Total	O	0	0
			160	160		
4	I	5	Total	O	0	0
			5	5		
4	L	25	Total	O	0	0
			25	25		

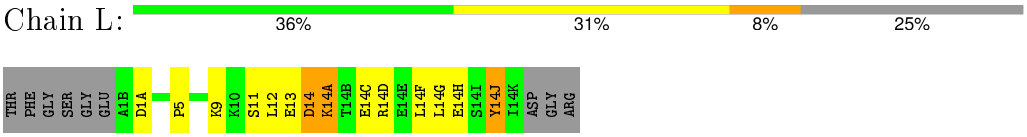
3 Residue-property plots (i)

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.

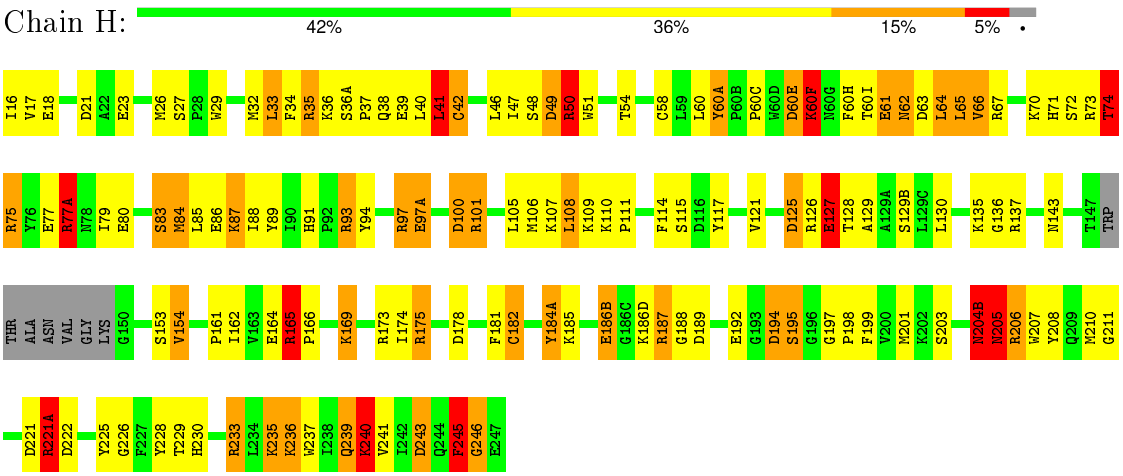
- Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L:



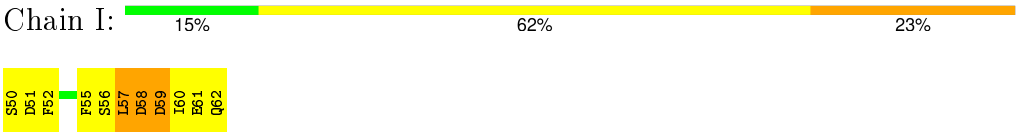
- Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

Chain H:



- Molecule 3: HIRULLIN

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	71.43Å 72.32Å 72.81Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2541	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.96	0/211	2.34	12/282 (4.3%)
2	H	0.91	0/2083	2.37	101/2813 (3.6%)
3	I	0.94	0/112	2.42	4/148 (2.7%)
All	All	0.92	0/2406	2.37	117/3243 (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
2	H	0	1

There are no bond length outliers.

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	77(A)	ARG	NE-CZ-NH2	-19.84	110.38	120.30
2	H	165	ARG	NE-CZ-NH1	-17.20	111.70	120.30
2	H	187	ARG	NE-CZ-NH1	15.25	127.92	120.30
2	H	77(A)	ARG	NE-CZ-NH1	14.77	127.68	120.30
2	H	206	ARG	NE-CZ-NH2	-14.74	112.93	120.30
2	H	49	ASP	CB-CG-OD2	14.30	131.17	118.30
2	H	206	ARG	NE-CZ-NH1	14.29	127.45	120.30
2	H	73	ARG	NE-CZ-NH2	13.99	127.29	120.30
2	H	165	ARG	NE-CZ-NH2	12.93	126.77	120.30
2	H	175	ARG	CD-NE-CZ	12.86	141.60	123.60
2	H	225	TYR	CB-CG-CD1	-12.61	113.43	121.00
3	I	59	ASP	CB-CG-OD1	-11.97	107.52	118.30
2	H	175	ARG	NE-CZ-NH2	-11.89	114.35	120.30
2	H	221(A)	ARG	NE-CZ-NH1	-11.61	114.50	120.30
2	H	33	LEU	CA-CB-CG	11.55	141.88	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	97	ARG	NE-CZ-NH2	-10.97	114.82	120.30
3	I	59	ASP	CB-CG-OD2	10.36	127.63	118.30
2	H	101	ARG	NE-CZ-NH2	-10.14	115.23	120.30
2	H	243	ASP	CB-CG-OD1	10.08	127.37	118.30
2	H	125	ASP	CB-CG-OD1	10.03	127.33	118.30
1	L	14(J)	TYR	CA-C-O	-9.85	99.43	120.10
2	H	73	ARG	NE-CZ-NH1	-9.43	115.58	120.30
2	H	97	ARG	NE-CZ-NH1	-9.41	115.59	120.30
2	H	75	ARG	NE-CZ-NH2	-9.34	115.63	120.30
2	H	60(A)	TYR	CB-CG-CD1	-9.21	115.48	121.00
2	H	97	ARG	NH1-CZ-NH2	9.08	129.39	119.40
2	H	137	ARG	NE-CZ-NH1	-9.02	115.79	120.30
2	H	175	ARG	NE-CZ-NH1	8.99	124.79	120.30
2	H	165	ARG	CD-NE-CZ	-8.80	111.27	123.60
2	H	221(A)	ARG	NE-CZ-NH2	8.68	124.64	120.30
2	H	225	TYR	CB-CG-CD2	8.59	126.16	121.00
2	H	184(A)	TYR	CB-CG-CD1	-8.39	115.97	121.00
2	H	187	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	H	97	ARG	CD-NE-CZ	-8.33	111.94	123.60
2	H	35	ARG	CD-NE-CZ	-8.30	111.97	123.60
2	H	21	ASP	CB-CG-OD2	-8.26	110.87	118.30
2	H	60(E)	ASP	CB-CG-OD1	-8.22	110.90	118.30
2	H	228	TYR	CB-CG-CD2	8.19	125.91	121.00
2	H	186(B)	GLU	OE1-CD-OE2	-7.93	113.78	123.30
2	H	205	ASN	CB-CA-C	7.83	126.06	110.40
2	H	50	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	H	100	ASP	CB-CG-OD2	-7.82	111.27	118.30
2	H	93	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	H	173	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	H	194	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	L	14(G)	LEU	CB-CA-C	6.88	123.27	110.20
2	H	80	GLU	CG-CD-OE1	6.73	131.76	118.30
2	H	74	THR	OG1-CB-CG2	6.69	125.40	110.00
2	H	80	GLU	CG-CD-OE2	-6.67	104.96	118.30
2	H	153	SER	N-CA-CB	6.66	120.49	110.50
2	H	246	GLY	O-C-N	6.60	133.26	122.70
2	H	221(A)	ARG	CA-CB-CG	6.59	127.90	113.40
2	H	115	SER	N-CA-CB	-6.57	100.64	110.50
2	H	181	PHE	CB-CA-C	6.53	123.45	110.40
2	H	47	ILE	CB-CG1-CD1	6.50	132.09	113.90
1	L	1(A)	ASP	CB-CG-OD1	-6.36	112.58	118.30
2	H	233	ARG	CD-NE-CZ	6.33	132.47	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	204(B)	ASN	C-N-CA	6.33	137.53	121.70
2	H	137	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	L	14(G)	LEU	CB-CG-CD1	6.30	121.72	111.00
2	H	97(A)	GLU	OE1-CD-OE2	6.29	130.85	123.30
2	H	75	ARG	CA-CB-CG	-6.08	100.03	113.40
1	L	14(C)	GLU	CG-CD-OE1	-6.07	106.16	118.30
2	H	27	SER	N-CA-CB	-6.04	101.44	110.50
2	H	243	ASP	CA-CB-CG	6.01	126.62	113.40
2	H	49	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	L	14(J)	TYR	CA-C-N	5.97	130.35	117.20
2	H	61	GLU	OE1-CD-OE2	-5.97	116.14	123.30
2	H	66	VAL	CA-CB-CG1	5.96	119.84	110.90
1	L	1(A)	ASP	N-CA-CB	-5.95	99.89	110.60
2	H	77	GLU	C-N-CA	5.86	136.34	121.70
2	H	67	ARG	NE-CZ-NH2	5.83	123.22	120.30
2	H	61	GLU	CG-CD-OE1	5.71	129.72	118.30
2	H	206	ARG	CD-NE-CZ	5.71	131.59	123.60
2	H	60(A)	TYR	CA-CB-CG	-5.68	102.61	113.40
2	H	125	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	H	245	PHE	C-N-CA	-5.66	110.41	122.30
2	H	60(F)	LYS	N-CA-CB	5.65	120.77	110.60
1	L	14(C)	GLU	CG-CD-OE2	5.59	129.48	118.30
2	H	117	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	H	73	ARG	CA-C-O	5.57	131.81	120.10
2	H	127	GLU	CA-CB-CG	5.56	125.63	113.40
2	H	208	TYR	CB-CG-CD1	-5.54	117.68	121.00
2	H	42	CYS	C-N-CA	5.53	133.92	122.30
2	H	240	LYS	N-CA-CB	-5.53	100.65	110.60
2	H	239	GLN	CA-C-O	5.52	131.69	120.10
2	H	97(A)	GLU	CG-CD-OE2	-5.51	107.29	118.30
2	H	127	GLU	CB-CG-CD	5.51	129.06	114.20
2	H	41	LEU	CB-CA-C	5.50	120.65	110.20
2	H	50	ARG	N-CA-CB	-5.49	100.72	110.60
2	H	108	LEU	CA-CB-CG	5.49	127.92	115.30
2	H	65	LEU	CB-CG-CD1	5.43	120.23	111.00
2	H	164	GLU	CA-CB-CG	5.42	125.33	113.40
2	H	184(A)	TYR	CB-CG-CD2	5.40	124.24	121.00
1	L	14(J)	TYR	CG-CD2-CE2	5.38	125.60	121.30
2	H	89	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	H	178	ASP	CB-CG-OD2	-5.38	113.46	118.30
2	H	60(A)	TYR	CB-CG-CD2	5.37	124.22	121.00
2	H	195	SER	CB-CA-C	5.35	120.27	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	198	PRO	CB-CA-C	-5.33	98.67	112.00
2	H	207	TRP	N-CA-CB	5.33	120.20	110.60
2	H	67	ARG	CD-NE-CZ	5.30	131.02	123.60
1	L	11	SER	CB-CA-C	5.28	120.12	110.10
2	H	186(D)	LYS	N-CA-C	-5.26	96.79	111.00
2	H	197	GLY	CA-C-O	5.24	130.03	120.60
3	I	57	LEU	CB-CA-C	5.23	120.14	110.20
3	I	55	PHE	O-C-N	5.22	131.05	122.70
1	L	14	ASP	CB-CA-C	5.19	120.79	110.40
1	L	13	GLU	OE1-CD-OE2	5.16	129.49	123.30
2	H	74	THR	N-CA-CB	-5.11	100.58	110.30
2	H	84	MET	CA-CB-CG	-5.09	104.65	113.30
2	H	165	ARG	CB-CG-CD	5.07	124.79	111.60
2	H	97(A)	GLU	N-CA-CB	-5.05	101.50	110.60
2	H	41	LEU	CB-CG-CD1	5.03	119.55	111.00
2	H	60	LEU	CB-CG-CD2	-5.01	102.48	111.00
2	H	54	THR	CA-CB-CG2	5.00	119.41	112.40
2	H	154	VAL	N-CA-CB	-5.00	100.50	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	77(A)	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	209	0	203	12	0
2	H	2031	0	2000	127	0
3	I	111	0	87	14	0
4	H	160	0	0	10	0
4	I	5	0	0	1	0
4	L	25	0	0	3	0
All	All	2541	0	2290	144	0

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 31.

All (144) 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:240:LYS:NZ	2:H:240:LYS:HB3	1.41	1.18
2:H:26:MET:HE1	4:H:501:HOH:O	1.57	1.04
2:H:240:LYS:HZ3	2:H:240:LYS:HB3	0.89	1.02
2:H:221(A):ARG:HH11	2:H:221(A):ARG:HG3	1.21	1.02
2:H:240:LYS:CB	2:H:240:LYS:NZ	2.26	0.95
2:H:205:ASN:HB2	4:H:670:HOH:O	1.66	0.94
2:H:185:LYS:N	2:H:186(B):GLU:OE1	2.00	0.94
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	1.70	0.92
1:L:9:LYS:HD3	4:L:534:HOH:O	1.68	0.91
1:L:14(A):LYS:HD3	2:H:23:GLU:CD	1.91	0.90
3:I:50:SER:O	3:I:52:PHE:N	2.07	0.87
3:I:62:GLN:OXT	4:I:690:HOH:O	1.94	0.85
2:H:221(A):ARG:HG3	2:H:221(A):ARG:NH1	1.89	0.85
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.81	0.81
2:H:199:PHE:HE1	2:H:201:MET:HE2	1.47	0.79
2:H:201:MET:CE	2:H:210:MET:HG3	2.15	0.76
2:H:60(I):THR:OG1	2:H:62:ASN:ND2	2.18	0.76
2:H:169:LYS:HE3	4:H:766:HOH:O	1.87	0.74
1:L:9:LYS:CD	4:L:534:HOH:O	2.30	0.74
2:H:199:PHE:HE1	2:H:201:MET:CE	2.01	0.73
1:L:14(D):ARG:O	1:L:14(H):GLU:HG3	1.89	0.72
2:H:204(B):ASN:HD22	2:H:205:ASN:N	1.89	0.71
2:H:36:LYS:O	2:H:38:GLN:HG2	1.90	0.71
2:H:126:ARG:NH1	2:H:126:ARG:HB2	2.05	0.71
2:H:240:LYS:CB	2:H:240:LYS:HZ3	1.85	0.71
2:H:187:ARG:NH1	2:H:221:ASP:O	2.23	0.71
2:H:85:LEU:HD13	2:H:106:MET:CE	2.21	0.69
2:H:162:ILE:HD11	2:H:199:PHE:CZ	2.28	0.68
2:H:35:ARG:HB2	2:H:41:LEU:HD13	1.75	0.68
2:H:35:ARG:NH1	2:H:39:GLU:OE2	2.24	0.67
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	1.97	0.67
2:H:50:ARG:NH1	2:H:86:GLU:OE1	2.28	0.67
1:L:14(A):LYS:HD3	2:H:23:GLU:OE1	1.94	0.66
2:H:85:LEU:CD1	2:H:106:MET:HE1	2.26	0.66
3:I:62:GLN:OE1	3:I:62:GLN:HA	1.96	0.66
3:I:50:SER:O	3:I:51:ASP:HB3	1.95	0.66
2:H:201:MET:HE1	2:H:210:MET:HG3	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:THR:HG22	2:H:75:ARG:HG3	1.78	0.65
2:H:36(A):SER:HA	2:H:37:PRO:C	2.17	0.64
1:L:14(A):LYS:CG	2:H:23:GLU:OE2	2.45	0.64
2:H:84:MET:HB2	2:H:109:LYS:HG3	1.80	0.63
2:H:97:ARG:HG3	4:H:416:HOH:O	1.98	0.62
2:H:49:ASP:HB3	2:H:114:PHE:CZ	2.34	0.62
2:H:162:ILE:HD11	2:H:199:PHE:HZ	1.65	0.61
2:H:35:ARG:O	2:H:38:GLN:HA	2.01	0.60
2:H:236:LYS:N	2:H:236:LYS:HD3	2.14	0.60
2:H:199:PHE:CE1	2:H:201:MET:HE2	2.35	0.60
2:H:126:ARG:HB3	2:H:127:GLU:OE1	2.03	0.59
3:I:50:SER:C	3:I:52:PHE:N	2.55	0.59
2:H:64:LEU:HD12	2:H:85:LEU:HD12	1.83	0.59
2:H:61:GLU:OE2	2:H:88:ILE:N	2.33	0.59
2:H:50:ARG:HD2	2:H:108:LEU:O	2.03	0.58
2:H:62:ASN:ND2	2:H:63:ASP:OD1	2.37	0.58
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.85	0.57
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.40	0.56
2:H:235:LYS:HE3	2:H:239:GLN:OE1	2.06	0.56
2:H:126:ARG:CB	2:H:126:ARG:NH1	2.68	0.56
2:H:77(A):ARG:HD3	4:H:444:HOH:O	2.04	0.56
2:H:17:VAL:O	2:H:188:GLY:HA2	2.05	0.56
2:H:62:ASN:HD22	2:H:63:ASP:N	2.04	0.56
2:H:51:TRP:HZ2	2:H:246:GLY:HA3	1.71	0.56
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.88	0.56
2:H:126:ARG:CB	2:H:126:ARG:CZ	2.84	0.56
3:I:59:ASP:N	3:I:59:ASP:OD1	2.34	0.55
2:H:110:LYS:NZ	3:I:61:GLU:HG2	2.21	0.55
2:H:187:ARG:NH2	2:H:222:ASP:OD1	2.26	0.55
2:H:32:MET:HG3	2:H:40:LEU:CD1	2.37	0.55
2:H:204(B):ASN:ND2	2:H:204(B):ASN:C	2.60	0.55
1:L:14(A):LYS:CD	2:H:23:GLU:CD	2.72	0.55
2:H:85:LEU:HD13	2:H:106:MET:HE1	1.85	0.55
2:H:85:LEU:HD22	2:H:106:MET:HB3	1.88	0.55
2:H:26:MET:CE	4:H:501:HOH:O	2.35	0.54
2:H:38:GLN:NE2	4:H:513:HOH:O	2.39	0.54
2:H:203:SER:O	2:H:205:ASN:HA	2.08	0.54
2:H:188:GLY:O	2:H:189:ASP:HB2	2.07	0.54
2:H:18:GLU:HG3	2:H:187:ARG:HG3	1.89	0.54
2:H:62:ASN:ND2	2:H:63:ASP:N	2.56	0.53
2:H:58:CYS:O	2:H:60(F):LYS:HD2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.91	0.52
2:H:50:ARG:NH1	2:H:107:LYS:HE3	2.24	0.52
2:H:85:LEU:HD11	2:H:106:MET:HE1	1.90	0.51
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.45	0.51
2:H:16:ILE:N	2:H:194:ASP:OD2	2.44	0.51
2:H:64:LEU:HD12	2:H:85:LEU:CD1	2.40	0.51
2:H:205:ASN:ND2	2:H:205:ASN:C	2.63	0.51
3:I:56:SER:C	3:I:58:ASP:H	2.13	0.51
2:H:49:ASP:C	2:H:49:ASP:OD1	2.47	0.50
2:H:126:ARG:HH11	2:H:126:ARG:HB2	1.77	0.50
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.47	0.49
2:H:70:LYS:HE3	2:H:72:SER:O	2.13	0.49
2:H:201:MET:HE3	2:H:210:MET:HG3	1.95	0.49
2:H:221(A):ARG:HH11	2:H:221(A):ARG:CG	1.91	0.48
1:L:12:LEU:HB3	4:L:701:HOH:O	2.12	0.48
2:H:187:ARG:HB2	2:H:221:ASP:OD1	2.13	0.48
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	1.95	0.48
2:H:125:ASP:OD1	2:H:128:THR:CB	2.62	0.48
2:H:42:CYS:HB3	2:H:195:SER:O	2.15	0.47
2:H:87:LYS:HA	2:H:87:LYS:HD2	1.74	0.47
2:H:143:ASN:ND2	2:H:192:GLU:HB3	2.29	0.47
2:H:203:SER:HB3	2:H:204(B):ASN:HD21	1.80	0.47
2:H:165:ARG:N	2:H:166:PRO:HD2	2.30	0.47
2:H:237:TRP:O	2:H:240:LYS:HB2	2.15	0.46
2:H:46:LEU:HD11	2:H:48:SER:O	2.16	0.46
2:H:110:LYS:HZ2	3:I:61:GLU:CD	2.19	0.46
2:H:240:LYS:CB	2:H:240:LYS:HZ2	2.26	0.46
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.32	0.45
3:I:60:ILE:CG2	3:I:61:GLU:H	2.30	0.45
2:H:51:TRP:CZ2	2:H:246:GLY:HA3	2.52	0.45
2:H:174:ILE:HD12	2:H:174:ILE:N	2.32	0.44
2:H:236:LYS:NZ	4:H:772:HOH:O	2.51	0.44
2:H:49:ASP:O	2:H:111:PRO:HA	2.17	0.44
2:H:100:ASP:O	2:H:101:ARG:HB2	2.18	0.44
2:H:93:ARG:O	2:H:101:ARG:HD2	2.18	0.44
2:H:162:ILE:CD1	2:H:199:PHE:CZ	2.99	0.44
2:H:64:LEU:HD11	2:H:88:ILE:HD11	1.99	0.44
2:H:110:LYS:HZ3	3:I:61:GLU:HG2	1.81	0.43
2:H:241:VAL:O	2:H:245:PHE:HD1	2.01	0.43
2:H:94:TYR:HA	2:H:101:ARG:HB2	2.01	0.43
2:H:74:THR:CG2	2:H:75:ARG:HG3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:184(A):TYR:HA	2:H:186(B):GLU:OE1	2.18	0.43
2:H:236:LYS:O	2:H:240:LYS:HB2	2.19	0.43
3:I:56:SER:C	3:I:58:ASP:N	2.71	0.42
1:L:14(A):LYS:CD	2:H:23:GLU:OE2	2.68	0.42
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.19	0.42
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.17	0.42
2:H:60(H):PHE:HB3	2:H:64:LEU:HD21	2.01	0.41
3:I:60:ILE:HG22	3:I:61:GLU:H	1.86	0.41
2:H:241:VAL:HB	2:H:245:PHE:HE1	1.85	0.41
2:H:61:GLU:OE2	2:H:87:LYS:HA	2.20	0.41
2:H:129:ALA:O	2:H:130:LEU:HB2	2.21	0.41
3:I:57:LEU:HA	3:I:60:ILE:HD12	2.02	0.41
2:H:83:SER:HB3	4:H:564:HOH:O	2.21	0.41
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.55	0.41
2:H:105:LEU:HA	2:H:105:LEU:HD23	1.91	0.41
2:H:29:TRP:CG	2:H:121:VAL:HB	2.55	0.41
2:H:36(A):SER:HB2	4:H:538:HOH:O	2.21	0.41
2:H:182:CYS:HA	2:H:226:GLY:O	2.21	0.41
2:H:165:ARG:HH11	2:H:165:ARG:HD3	1.14	0.40
2:H:135:LYS:HA	2:H:161:PRO:HA	2.03	0.40
1:L:14(A):LYS:HG2	1:L:14(A):LYS:H	1.64	0.40
2:H:88:ILE:CD1	2:H:106:MET:HE3	2.51	0.40
2:H:211:GLY:HA2	2:H:229:THR:O	2.22	0.40
2:H:230:HIS:ND1	2:H:233:ARG:HG3	2.36	0.40
2:H:60(A):TYR:CZ	2:H:60(C):PRO:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	25/36 (69%)	23 (92%)	2 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	248/259 (96%)	234 (94%)	14 (6%)	0	100 100
3	I	11/13 (85%)	8 (73%)	3 (27%)	0	100 100
All	All	284/308 (92%)	265 (93%)	19 (7%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	23/31 (74%)	19 (83%)	4 (17%)	2 2
2	H	218/225 (97%)	191 (88%)	27 (12%)	6 6
3	I	13/13 (100%)	12 (92%)	1 (8%)	16 20
All	All	254/269 (94%)	222 (87%)	32 (13%)	5 5

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	ASP
1	L	14(A)	LYS
1	L	14(F)	LEU
1	L	14(J)	TYR
2	H	33	LEU
2	H	41	LEU
2	H	50	ARG
2	H	60(E)	ASP
2	H	60(F)	LYS
2	H	62	ASN
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	74	THR
2	H	77(A)	ARG
2	H	79	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	83	SER
2	H	87	LYS
2	H	127	GLU
2	H	129(B)	SER
2	H	165	ARG
2	H	169	LYS
2	H	182	CYS
2	H	204(B)	ASN
2	H	205	ASN
2	H	221(A)	ARG
2	H	235	LYS
2	H	236	LYS
2	H	240	LYS
2	H	243	ASP
2	H	245	PHE
3	I	58	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	62	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	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 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.