



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:06 PM UTC

PDB ID : 3T2N / pdb_00003t2n
Title : Human hepsin protease in complex with the Fab fragment of an inhibitory antibody
Authors : Koschubs, T.; Dengl, S.; Duerr, H.; Kaluza, K.; Georges, G.; Hartl, C.; Jennewein, S.; Lanzendoerfer, M.; Auer, J.; Stern, A.; Huang, K.-S.; Kostrewa, D.; Ries, S.; Hansen, S.; Kohnert, U.; Cramer, P.; Mundigl, O.
Deposited on : 2011-07-22
Resolution : 2.55 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

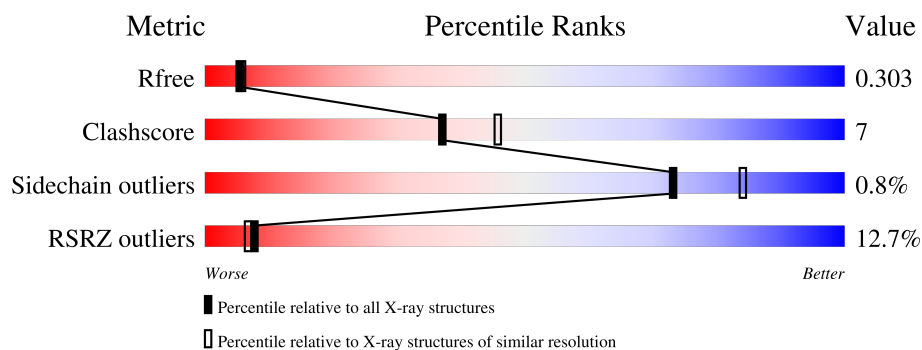
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 of 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	372	15% 74% 16% 9%
1	B	372	17% 74% 15% 10%
2	H	225	8% 75% 15% 10%
2	I	225	9% 78% 13% 9%
3	L	215	8% 79% 19% ..
3	M	215	7% 80% 18% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11749 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 Serine protease hepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2605	1638	470	478	19			
1	B	335	Total	C	N	O	S	0	0	0
			2576	1622	464	471	19			

- Molecule 2 is a protein called Antibody, Fab fragment, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	0	0
			1535	980	250	299	6			
2	I	205	Total	C	N	O	S	0	0	0
			1547	987	252	302	6			

- Molecule 3 is a protein called Antibody, Fab fragment, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1582	996	267	315	4			
3	M	212	Total	C	N	O	S	0	0	0
			1589	1000	268	317	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	74	Total	O	0	0
			74	74		
4	H	46	Total	O	0	0
			46	46		
4	I	36	Total	O	0	0
			36	36		

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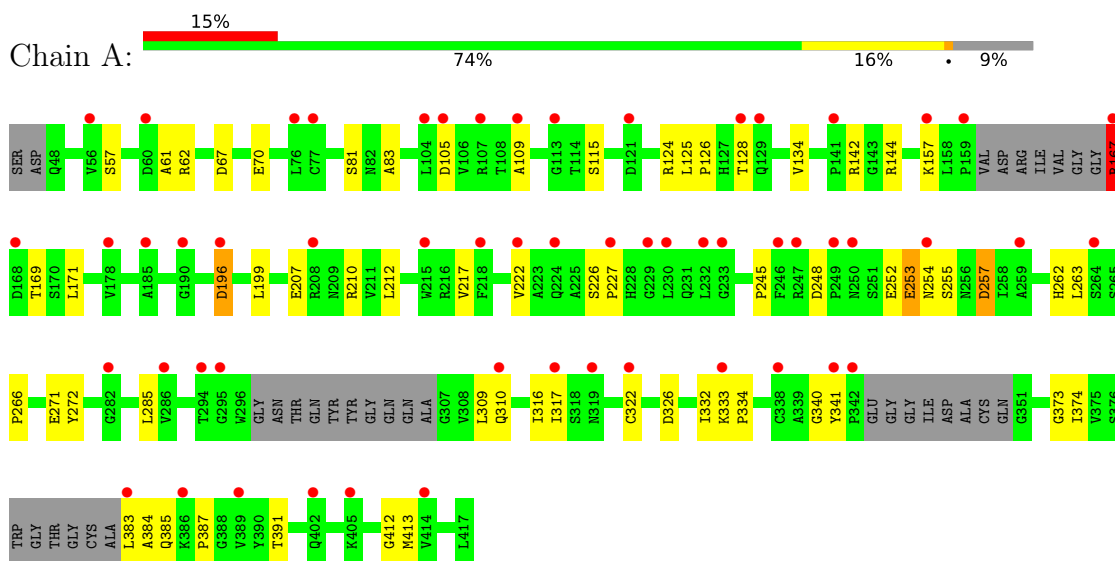
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	40	Total	O	0	0
			40	40		
4	M	55	Total	O	0	0
			55	55		

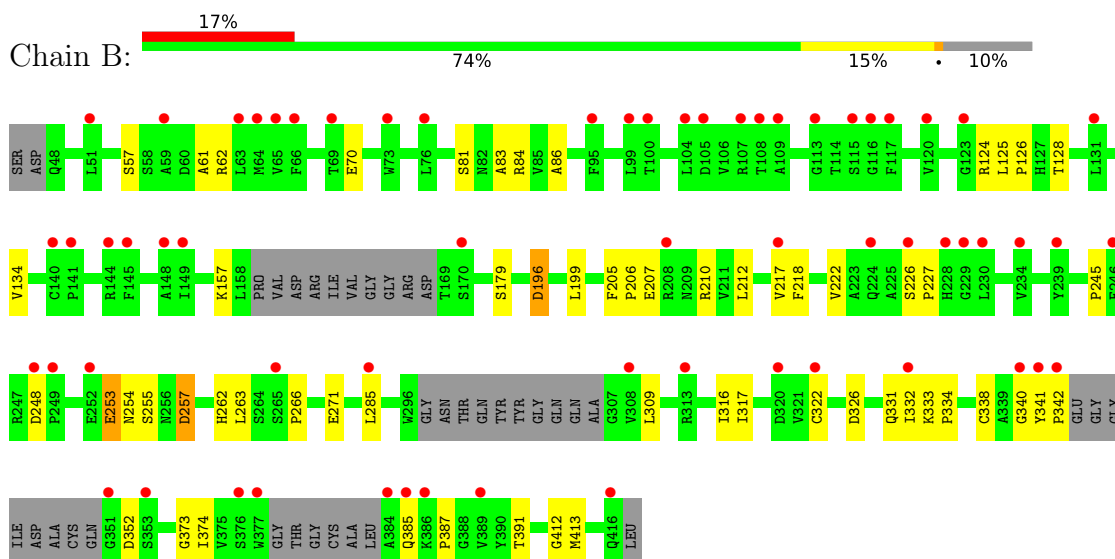
3 Residue-property plots [i](#)

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 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.

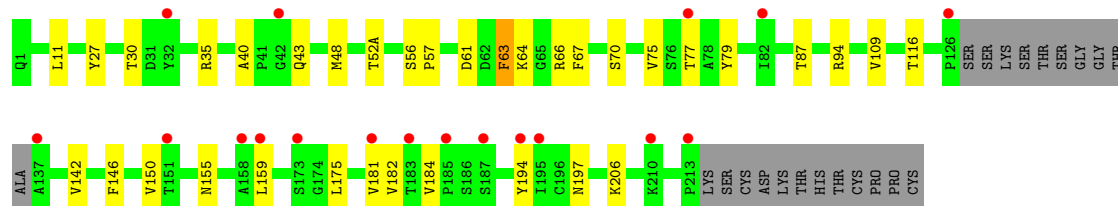
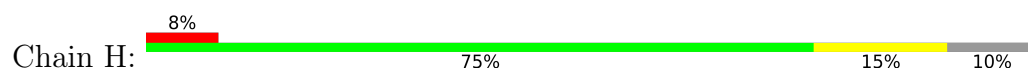
- Molecule 1: Serine protease hepsin



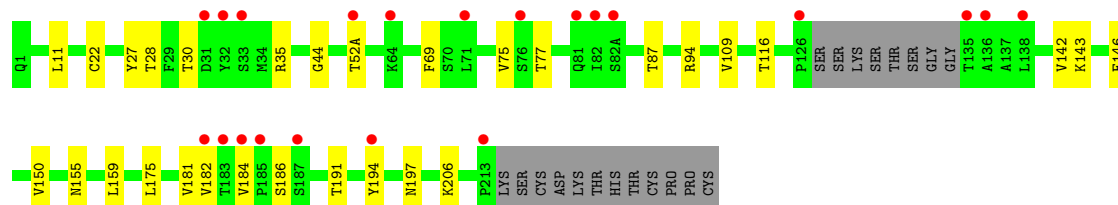
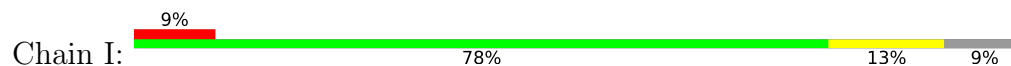
- Molecule 1: Serine protease hepsin



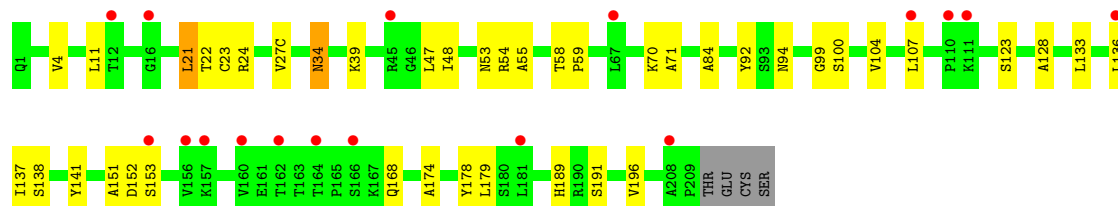
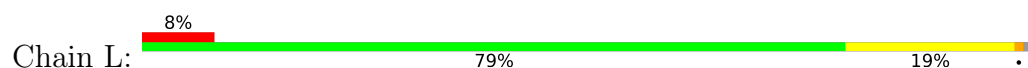
- Molecule 2: Antibody, Fab fragment, Heavy Chain



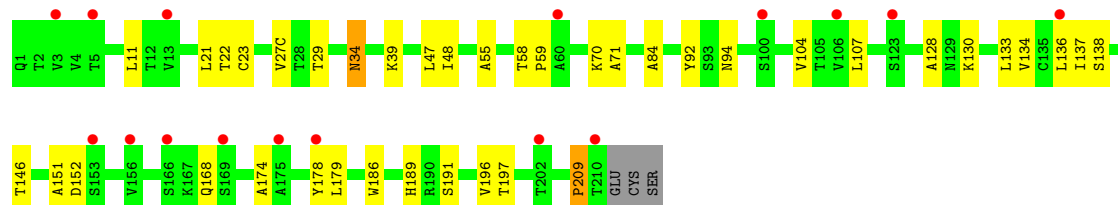
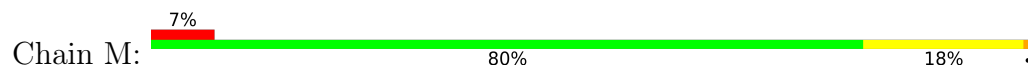
- Molecule 2: Antibody, Fab fragment, Heavy Chain



- Molecule 3: Antibody, Fab fragment, Light Chain



- Molecule 3: Antibody, Fab fragment, Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.98Å 66.58Å 108.33Å 88.71° 94.30° 104.53°	Depositor
Resolution (Å)	47.33 – 2.55 47.33 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.33-2.55) 98.7 (47.33-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.242 , 0.275 (Not available) , 0.303	Depositor DCC
R_{free} test set	2772 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	0.84	0/2665	1.28	14/3615 (0.4%)
1	B	0.87	2/2637 (0.1%)	1.29	20/3579 (0.6%)
2	H	0.82	0/1575	1.20	4/2148 (0.2%)
2	I	0.80	1/1587 (0.1%)	1.21	8/2165 (0.4%)
3	L	0.85	0/1623	1.23	10/2222 (0.5%)
3	M	0.85	0/1630	1.25	9/2232 (0.4%)
All	All	0.84	3/11717 (0.0%)	1.25	65/15961 (0.4%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	PHE	C-N	7.28	1.42	1.33
1	B	206	PRO	N-CD	-5.36	1.40	1.47
2	I	22	CYS	CA-C	-5.12	1.47	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	104	VAL	N-CA-CB	8.00	120.57	111.21
3	M	209	PRO	CA-C-N	7.39	135.00	121.70
3	M	209	PRO	C-N-CA	7.39	135.00	121.70
3	M	104	VAL	N-CA-CB	7.29	119.74	111.21
3	M	34	ASN	CA-CB-CG	7.27	119.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	PHE	CA-C-N	-7.04	113.06	120.03
1	B	205	PHE	C-N-CA	-7.04	113.06	120.03
3	L	34	ASN	CA-CB-CG	7.02	119.62	112.60
3	M	107	LEU	N-CA-C	6.73	119.40	108.63
1	A	253	GLU	N-CA-C	6.71	119.96	110.23
2	H	63	PHE	N-CA-C	6.50	120.52	112.59
1	B	254	ASN	N-CA-C	-6.41	105.76	113.97
1	B	254	ASN	CA-C-N	5.95	129.74	120.75
1	B	254	ASN	C-N-CA	5.95	129.74	120.75
1	A	196	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	196	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	207	GLU	CA-C-N	5.90	128.18	120.28
1	B	207	GLU	C-N-CA	5.90	128.18	120.28
3	L	153	SER	N-CA-C	-5.90	105.43	114.16
1	A	252	GLU	CA-C-N	5.88	129.06	120.71
1	A	252	GLU	C-N-CA	5.88	129.06	120.71
1	A	207	GLU	CA-C-N	5.84	128.11	120.28
1	A	207	GLU	C-N-CA	5.84	128.11	120.28
1	B	124	ARG	CA-C-N	5.83	127.38	120.09
1	B	124	ARG	C-N-CA	5.83	127.38	120.09
1	B	254	ASN	CA-CB-CG	5.79	118.39	112.60
2	H	66	ARG	N-CA-C	5.79	117.67	111.36
1	B	83	ALA	CA-C-N	5.61	127.73	120.44
1	B	83	ALA	C-N-CA	5.61	127.73	120.44
3	L	53	ASN	CA-CB-CG	5.57	118.17	112.60
1	B	352	ASP	CA-C-N	5.55	128.64	120.82
1	B	352	ASP	C-N-CA	5.55	128.64	120.82
3	L	59	PRO	CA-C-N	5.47	129.35	120.60
3	L	59	PRO	C-N-CA	5.47	129.35	120.60
3	M	128	ALA	CA-C-N	5.45	129.87	122.07
3	M	128	ALA	C-N-CA	5.45	129.87	122.07
1	B	86	ALA	CA-C-N	5.44	125.97	119.94
1	B	86	ALA	C-N-CA	5.44	125.97	119.94
1	A	124	ARG	CA-C-N	5.43	126.88	120.09
1	A	124	ARG	C-N-CA	5.43	126.88	120.09
1	A	167	ARG	CD-NE-CZ	5.42	131.99	124.40
2	I	155	ASN	CA-C-N	5.41	129.82	122.19
2	I	155	ASN	C-N-CA	5.41	129.82	122.19
3	M	59	PRO	CA-C-N	5.41	129.26	120.60
3	M	59	PRO	C-N-CA	5.41	129.26	120.60
1	A	81	SER	CA-C-N	5.41	127.52	120.28
1	A	81	SER	C-N-CA	5.41	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	186	SER	CA-C-N	5.37	128.21	120.38
2	I	186	SER	C-N-CA	5.37	128.21	120.38
2	I	69	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	83	ALA	CA-C-N	5.29	127.32	120.44
1	A	83	ALA	C-N-CA	5.29	127.32	120.44
3	L	123	SER	CA-C-N	5.24	127.25	120.44
3	L	123	SER	C-N-CA	5.24	127.25	120.44
3	L	128	ALA	CA-C-N	5.23	129.55	122.07
3	L	128	ALA	C-N-CA	5.23	129.55	122.07
2	H	155	ASN	CA-C-N	5.21	129.53	122.19
2	H	155	ASN	C-N-CA	5.21	129.53	122.19
2	I	191	THR	N-CA-C	-5.14	107.67	114.04
2	I	28	THR	CA-C-N	5.14	127.42	120.38
2	I	28	THR	C-N-CA	5.14	127.42	120.38
1	B	352	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	257	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	257	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	253	GLU	N-CA-C	5.01	117.49	110.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	B	257	ASP	Sidechain

5.2 Too-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 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	A	2605	0	2536	44	0
1	B	2576	0	2500	38	0
2	H	1535	0	1502	22	0
2	I	1547	0	1514	16	0
3	L	1582	0	1541	25	0
3	M	1589	0	1548	27	0
4	A	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	74	0	0	0	0
4	H	46	0	0	0	0
4	I	36	0	0	0	0
4	L	40	0	0	1	0
4	M	55	0	0	1	0
All	All	11749	0	11141	160	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 7.

All (160) 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)
1:B:317:ILE:HD11	1:B:340:GLY:HA2	1.52	0.92
2:I:181:VAL:HG11	3:M:136:LEU:HD13	1.54	0.89
1:A:383:LEU:O	1:A:383:LEU:HG	1.76	0.85
2:H:75:VAL:HG13	2:H:77:THR:HG22	1.66	0.77
2:H:181:VAL:HG11	3:L:136:LEU:HD13	1.66	0.76
1:A:383:LEU:HD21	3:L:54:ARG:H	1.51	0.74
2:I:75:VAL:HG13	2:I:77:THR:HG22	1.70	0.73
1:A:169:THR:HG22	1:A:222:VAL:HG21	1.70	0.71
3:L:47:LEU:HD22	3:L:58:THR:HG22	1.76	0.67
1:A:317:ILE:HD11	1:A:340:GLY:HA2	1.77	0.67
2:I:181:VAL:CG1	3:M:136:LEU:HD13	2.24	0.67
2:H:67:PHE:CD1	2:H:67:PHE:N	2.63	0.65
3:M:47:LEU:HD22	3:M:58:THR:HG22	1.77	0.65
1:B:338:CYS:SG	1:B:387:PRO:HB2	2.37	0.65
2:H:61:ASP:OD1	2:H:64:LYS:NZ	2.28	0.64
3:M:134:VAL:HG12	3:M:136:LEU:HD21	1.78	0.64
1:A:105:ASP:O	1:A:109:ALA:HB3	1.99	0.63
3:L:100:SER:HB2	4:L:225:HOH:O	1.97	0.62
2:H:61:ASP:HA	2:H:64:LYS:HD2	1.80	0.62
1:B:196:ASP:O	1:B:262:HIS:HD2	1.83	0.62
1:A:169:THR:HG22	1:A:222:VAL:CG2	2.31	0.60
1:A:196:ASP:O	1:A:262:HIS:HD2	1.84	0.60
1:B:84:ARG:HB2	1:B:125:LEU:HD21	1.83	0.60
3:M:151:ALA:O	3:M:191:SER:O	2.21	0.59
3:L:151:ALA:O	3:L:191:SER:O	2.20	0.59
3:M:23:CYS:HB3	3:M:71:ALA:HB3	1.84	0.59
3:L:23:CYS:HB3	3:L:71:ALA:HB3	1.84	0.58
3:L:168:GLN:HE21	3:L:174:ALA:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:168:GLN:HE21	3:M:174:ALA:HB2	1.68	0.58
1:B:222:VAL:CG2	1:B:309:LEU:HB3	2.34	0.58
1:A:383:LEU:HD21	3:L:54:ARG:N	2.19	0.57
3:M:11:LEU:HD12	3:M:21:LEU:HD22	1.86	0.57
1:A:322:CYS:HB2	1:A:332:ILE:HD11	1.86	0.57
1:B:341:TYR:CD2	3:M:29:THR:HG21	2.40	0.57
1:A:105:ASP:O	1:A:109:ALA:CB	2.53	0.57
1:B:322:CYS:HB2	1:B:332:ILE:HD11	1.87	0.57
2:H:181:VAL:CG1	3:L:136:LEU:HD13	2.33	0.57
3:L:11:LEU:HD12	3:L:21:LEU:HD22	1.87	0.56
1:B:341:TYR:O	1:B:342:PRO:C	2.48	0.55
1:A:222:VAL:CG2	1:A:309:LEU:HB3	2.37	0.55
3:L:55:ALA:HB3	3:L:58:THR:HG23	1.89	0.55
1:B:210:ARG:HE	1:B:413:MET:HE2	1.72	0.55
1:A:142:ARG:HG2	1:A:144:ARG:HG3	1.89	0.55
3:M:152:ASP:OD2	3:M:189:HIS:HD2	1.91	0.54
3:M:55:ALA:HB3	3:M:58:THR:HG23	1.89	0.54
1:A:333:LYS:HB3	1:A:334:PRO:HD2	1.90	0.54
1:A:128:THR:HG21	1:A:134:VAL:HG11	1.89	0.54
2:I:197:ASN:HB3	2:I:206:LYS:HE2	1.90	0.53
3:M:134:VAL:CG1	3:M:136:LEU:HD21	2.38	0.53
1:A:210:ARG:HE	1:A:413:MET:HE2	1.72	0.53
1:B:333:LYS:HB3	1:B:334:PRO:HD2	1.90	0.53
3:M:138:SER:HB2	3:M:168:GLN:HE22	1.74	0.53
2:H:27:TYR:CZ	2:H:94:ARG:HD2	2.44	0.52
2:H:146:PHE:HB2	2:H:175:LEU:HD23	1.90	0.52
1:A:373:GLY:HA2	1:A:391:THR:O	2.10	0.52
2:H:67:PHE:HD1	2:H:67:PHE:H	1.56	0.52
2:H:197:ASN:HB3	2:H:206:LYS:HE2	1.91	0.52
1:A:167:ARG:O	1:A:310:GLN:HA	2.10	0.52
1:B:385:GLN:HB3	3:M:29:THR:HG23	1.92	0.51
2:I:27:TYR:CZ	2:I:94:ARG:HD2	2.45	0.51
1:B:222:VAL:HG22	1:B:309:LEU:HB3	1.93	0.51
2:I:146:PHE:HB2	2:I:175:LEU:HD23	1.92	0.51
3:M:92:TYR:O	3:M:94:ASN:N	2.41	0.51
3:M:137:ILE:HG12	3:M:196:VAL:HG21	1.92	0.51
1:A:326:ASP:O	2:H:35:ARG:NH2	2.43	0.51
1:B:373:GLY:HA2	1:B:391:THR:O	2.11	0.51
3:M:22:THR:HB	3:M:70:LYS:HD2	1.92	0.50
2:I:30:THR:HA	2:I:52(A):THR:HG22	1.93	0.50
1:B:57:SER:HB2	1:B:62:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD12	1:B:412:GLY:HA2	1.94	0.50
1:B:128:THR:HG21	1:B:134:VAL:HG11	1.93	0.50
1:B:157:LYS:HB2	1:B:271:GLU:HA	1.94	0.50
1:B:326:ASP:O	2:I:35:ARG:NH2	2.44	0.50
1:A:125:LEU:N	1:A:126:PRO:HD2	2.27	0.50
2:I:87:THR:HA	2:I:109:VAL:O	2.12	0.50
3:L:22:THR:HB	3:L:70:LYS:HD2	1.93	0.50
3:L:152:ASP:OD2	3:L:189:HIS:HD2	1.95	0.49
1:A:57:SER:HB2	1:A:62:ARG:HG2	1.94	0.49
3:L:138:SER:HB2	3:L:168:GLN:HE22	1.77	0.49
1:B:317:ILE:HD12	1:B:387:PRO:HB3	1.95	0.49
2:I:143:LYS:NZ	3:M:130:LYS:HD2	2.27	0.49
1:A:245:PRO:HA	1:A:248:ASP:O	2.12	0.48
2:H:87:THR:HA	2:H:109:VAL:O	2.13	0.48
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.47	0.48
3:L:107:LEU:HD23	3:L:141:TYR:HE1	1.78	0.48
2:I:184:VAL:HG11	2:I:194:TYR:CE1	2.48	0.48
1:A:383:LEU:O	1:A:384:ALA:HB2	2.13	0.48
2:H:11:LEU:HD11	2:H:146:PHE:HZ	1.78	0.48
2:H:30:THR:HA	2:H:52(A):THR:HG22	1.94	0.48
2:H:70:SER:OG	2:H:79:TYR:HB2	2.13	0.48
1:A:212:LEU:HD12	1:A:412:GLY:HA2	1.94	0.48
1:A:341:TYR:HE2	1:A:385:GLN:HE21	1.61	0.47
3:L:137:ILE:HG12	3:L:196:VAL:HG21	1.95	0.47
1:B:245:PRO:HA	1:B:248:ASP:O	2.15	0.47
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.97	0.47
1:B:81:SER:HB2	1:B:84:ARG:HD3	1.96	0.47
1:B:285:LEU:HG	1:B:316:ILE:HD13	1.97	0.47
3:L:92:TYR:O	3:L:94:ASN:N	2.43	0.47
2:I:11:LEU:HD11	2:I:146:PHE:HZ	1.80	0.46
1:B:341:TYR:HE2	1:B:385:GLN:HE21	1.63	0.46
2:H:142:VAL:HG11	2:H:150:VAL:HG11	1.97	0.46
1:A:222:VAL:HG23	1:A:309:LEU:HB3	1.97	0.46
1:B:196:ASP:HB3	1:B:266:PRO:HA	1.98	0.46
1:A:222:VAL:HG22	1:A:309:LEU:HB3	1.98	0.46
3:L:47:LEU:HA	3:L:58:THR:HG21	1.98	0.46
1:B:317:ILE:CD1	1:B:340:GLY:HA2	2.36	0.46
1:A:115:SER:HB2	1:B:70:GLU:O	2.15	0.46
1:B:253:GLU:HG3	1:B:255:SER:H	1.81	0.45
3:L:39:LYS:HG2	3:L:84:ALA:HB2	1.98	0.45
1:A:196:ASP:HB3	1:A:266:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:HG3	1:A:255:SER:N	2.31	0.45
1:B:222:VAL:HG23	1:B:309:LEU:HB3	1.97	0.45
1:A:157:LYS:HB2	1:A:271:GLU:HA	1.98	0.45
1:B:199:LEU:HD21	1:B:374:ILE:HD11	1.98	0.45
1:B:125:LEU:N	1:B:126:PRO:HD2	2.32	0.44
1:B:199:LEU:CD2	1:B:374:ILE:HD11	2.46	0.44
1:A:67:ASP:OD2	1:A:70:GLU:HB2	2.17	0.44
2:I:142:VAL:HG11	2:I:150:VAL:HG11	2.00	0.44
2:I:159:LEU:HD21	2:I:182:VAL:HG21	2.00	0.44
1:A:105:ASP:HB2	1:A:144:ARG:HH11	1.83	0.44
1:A:285:LEU:HG	1:A:316:ILE:HD13	1.98	0.44
1:A:383:LEU:O	1:A:383:LEU:CG	2.52	0.44
3:L:24:ARG:HB2	3:L:70:LYS:HD3	2.00	0.44
3:M:186:TRP:O	3:M:209:PRO:HG3	2.17	0.44
1:A:199:LEU:CD2	1:A:374:ILE:HD11	2.48	0.43
1:B:253:GLU:HG3	1:B:255:SER:N	2.32	0.43
2:H:48:MET:HG2	2:H:63:PHE:CZ	2.53	0.43
1:A:142:ARG:CG	1:A:144:ARG:HG3	2.49	0.43
1:A:254:ASN:O	1:A:257:ASP:HB2	2.17	0.43
1:A:317:ILE:HD12	1:A:387:PRO:HB3	2.01	0.43
2:H:40:ALA:O	2:H:43:GLN:HB2	2.18	0.43
1:B:179:SER:HB3	1:B:218:PHE:HB3	2.01	0.43
1:B:217:VAL:HG21	1:B:263:LEU:CD2	2.48	0.43
1:B:217:VAL:HG21	1:B:263:LEU:HD22	2.00	0.43
2:I:44:GLY:HA3	4:M:216:HOH:O	2.19	0.42
3:M:133:LEU:HD12	3:M:179:LEU:HD23	2.01	0.42
1:B:226:SER:HA	1:B:227:PRO:HD3	1.90	0.42
3:M:133:LEU:O	3:M:178:TYR:HA	2.19	0.42
3:M:39:LYS:HG2	3:M:84:ALA:HB2	2.01	0.42
2:H:159:LEU:HD21	2:H:182:VAL:HG21	2.00	0.42
1:A:226:SER:HA	1:A:227:PRO:HD3	1.92	0.42
1:A:171:LEU:HD22	1:A:272:TYR:CD1	2.55	0.42
2:H:56:SER:HA	2:H:57:PRO:HD3	1.97	0.42
3:L:133:LEU:O	3:L:178:TYR:HA	2.19	0.42
1:B:331:GLN:HE21	1:B:331:GLN:HB2	1.69	0.42
3:M:34:ASN:HA	3:M:48:ILE:O	2.20	0.42
3:M:47:LEU:HA	3:M:58:THR:HG21	2.02	0.42
2:H:116:THR:HA	2:H:146:PHE:O	2.20	0.42
1:A:57:SER:O	1:A:61:ALA:HA	2.19	0.41
1:A:217:VAL:HG21	1:A:263:LEU:CD2	2.50	0.41
3:L:27(C):VAL:HG11	3:L:71:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:HG21	1:A:263:LEU:HD22	2.03	0.41
1:B:57:SER:O	1:B:61:ALA:HA	2.21	0.41
3:L:34:ASN:HA	3:L:48:ILE:O	2.20	0.41
3:M:152:ASP:OD2	3:M:189:HIS:CD2	2.72	0.41
3:M:146:THR:HB	3:M:197:THR:HB	2.02	0.41
1:A:199:LEU:HD21	1:A:374:ILE:HD11	2.02	0.41
3:L:4:VAL:O	3:L:99:GLY:HA2	2.22	0.40
3:M:27(C):VAL:HG11	3:M:71:ALA:HB2	2.02	0.40
2:I:116:THR:HA	2:I:146:PHE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	A	21/302 (7%)	21 (100%)	0	100	100
2	I	18/191 (9%)	18 (100%)	0	100	100
3	L	83/179 (46%)	82 (99%)	1 (1%)	63	78
All	All	122/672 (18%)	121 (99%)	1 (1%)	73	84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
3	L	168	GLN
3	L	189	HIS
3	L	195	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/372 (91%)	1.23	56 (16%) 4 3	25, 48, 72, 93	1 (0%)
1	B	335/372 (90%)	1.27	63 (18%) 3 2	28, 49, 72, 102	1 (0%)
2	H	203/225 (90%)	1.03	18 (8%) 15 14	25, 45, 68, 88	0
2	I	205/225 (91%)	1.01	21 (10%) 12 11	25, 44, 67, 88	0
3	L	211/215 (98%)	0.98	17 (8%) 18 17	24, 44, 61, 79	0
3	M	212/215 (98%)	0.94	16 (7%) 20 19	30, 43, 58, 64	0
All	All	1505/1624 (92%)	1.11	191 (12%) 8 7	24, 46, 69, 102	2 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	42	GLY	4.8
1	A	222	VAL	4.8
1	A	168	ASP	4.5
1	B	59	ALA	4.5
1	A	383	LEU	4.3
2	I	183	THR	4.0
1	B	224	GLN	4.0
1	B	141	PRO	3.8
1	A	233	GLY	3.6
1	B	123	GLY	3.5
1	B	104	LEU	3.4
1	B	230	LEU	3.4
1	A	386	LYS	3.3
2	H	194	TYR	3.3
1	B	148	ALA	3.2
1	A	259	ALA	3.2
3	M	153	SER	3.2
2	H	159	LEU	3.2
2	I	194	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	105	ASP	3.1
1	B	252	GLU	3.1
1	B	322	CYS	3.0
1	A	224	GLN	3.0
3	L	156	VAL	3.0
1	B	107	ARG	2.9
1	B	239	TYR	2.9
2	H	213	PRO	2.9
3	M	210	THR	2.9
2	H	195	ILE	2.8
2	I	187	SER	2.8
3	L	160	VAL	2.8
1	A	249	PRO	2.8
1	A	342	PRO	2.8
2	H	126	PRO	2.8
2	H	158	ALA	2.8
1	A	129	GLN	2.8
1	B	66	PHE	2.8
2	I	136	ALA	2.8
1	A	60	ASP	2.8
2	I	182	VAL	2.8
3	M	13	VAL	2.8
1	B	246	PHE	2.8
1	A	141	PRO	2.7
1	B	342	PRO	2.7
3	L	164	THR	2.7
1	B	100	THR	2.7
1	A	229	GLY	2.7
1	B	265	SER	2.7
1	B	376	SER	2.7
1	A	294	THR	2.7
1	B	113	GLY	2.7
3	L	111	LYS	2.7
3	L	153	SER	2.7
3	L	162	THR	2.7
1	A	56	VAL	2.6
1	A	128	THR	2.6
1	A	341	TYR	2.6
1	B	377	TRP	2.6
3	L	157	LYS	2.6
2	I	185	PRO	2.6
3	M	136	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	81	GLN	2.6
1	A	218	PHE	2.6
1	B	353	SER	2.6
3	M	166	SER	2.6
3	M	178	TYR	2.6
1	A	107	ARG	2.5
1	B	208	ARG	2.5
1	A	414	VAL	2.5
1	B	416	GLN	2.5
3	M	3	VAL	2.5
3	M	123	SER	2.5
3	L	16	GLY	2.5
1	B	95	PHE	2.5
2	H	77	THR	2.5
1	A	113	GLY	2.5
1	B	340	GLY	2.5
1	A	317	ILE	2.5
1	B	332	ILE	2.5
1	A	230	LEU	2.5
1	B	51	LEU	2.5
1	A	167	ARG	2.5
2	I	135	THR	2.5
1	B	351	GLY	2.5
1	A	178	VAL	2.5
1	B	313	ARG	2.5
2	H	151	THR	2.5
2	H	173	SER	2.5
1	B	63	LEU	2.4
1	B	99	LEU	2.4
3	L	136	LEU	2.4
1	B	116	GLY	2.4
2	I	82(A)	SER	2.4
1	A	250	ASN	2.4
1	B	108	THR	2.4
1	A	196	ASP	2.4
1	A	254	ASN	2.4
1	A	159	PRO	2.3
1	A	402	GLN	2.3
1	B	76	LEU	2.3
2	I	31	ASP	2.3
1	A	227	PRO	2.3
3	M	202	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	33	SER	2.3
1	A	246	PHE	2.3
3	M	156	VAL	2.3
3	M	175	ALA	2.3
1	A	310	GLN	2.3
2	I	64	LYS	2.3
1	B	120	VAL	2.3
1	B	217	VAL	2.3
2	I	184	VAL	2.3
1	B	249	PRO	2.3
2	I	126	PRO	2.3
3	L	110	PRO	2.3
1	B	170	SER	2.3
2	I	76	SER	2.3
1	B	73	TRP	2.3
1	B	248	ASP	2.3
2	H	32	TYR	2.3
2	I	52(A)	THR	2.2
1	B	105	ASP	2.2
1	A	389	VAL	2.2
2	H	185	PRO	2.2
1	B	109	ALA	2.2
2	H	137	ALA	2.2
1	B	226	SER	2.2
1	A	286	VAL	2.2
1	A	322	CYS	2.2
1	B	140	CYS	2.2
1	B	341	TYR	2.2
3	L	181	LEU	2.2
1	B	145	PHE	2.2
1	A	109	ALA	2.2
1	A	157	LYS	2.2
1	A	77	CYS	2.2
1	B	229	GLY	2.2
3	L	107	LEU	2.2
2	H	82	ILE	2.2
3	L	45	ARG	2.2
1	B	384	ALA	2.1
1	B	385	GLN	2.1
1	B	131	LEU	2.1
1	A	208	ARG	2.1
1	A	247	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	264	SER	2.1
1	B	115	SER	2.1
1	B	320	ASP	2.1
1	B	228	HIS	2.1
1	B	389	VAL	2.1
1	B	285	LEU	2.1
3	L	12	THR	2.1
2	I	32	TYR	2.1
3	L	166	SER	2.1
1	B	65	VAL	2.1
1	B	308	VAL	2.1
2	H	181	VAL	2.1
3	M	106	VAL	2.1
1	A	185	ALA	2.1
1	A	215	TRP	2.1
2	I	71	LEU	2.1
2	I	138	LEU	2.1
1	B	144	ARG	2.1
1	A	121	ASP	2.1
1	A	333	LYS	2.1
1	B	386	LYS	2.1
3	L	208	ALA	2.1
3	M	5	THR	2.1
1	B	149	ILE	2.1
2	I	82	ILE	2.1
2	H	187	SER	2.1
3	M	100	SER	2.1
3	M	169	SER	2.1
1	B	64	MET	2.1
1	B	234	VAL	2.0
3	M	60	ALA	2.0
1	A	232	LEU	2.0
1	A	190	GLY	2.0
2	H	210	LYS	2.0
2	I	213	PRO	2.0
1	A	338	CYS	2.0
1	B	117	PHE	2.0
1	A	76	LEU	2.0
1	A	104	LEU	2.0
3	L	67	LEU	2.0
1	A	282	GLY	2.0
1	A	295	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASN	2.0
1	A	405	LYS	2.0
1	B	69	THR	2.0
2	H	183	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.