



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:39 AM BST

PDB ID : 1IGF  
Title : CRYSTAL STRUCTURES OF AN ANTIBODY TO A PEPTIDE AND ITS COMPLEX WITH PEPTIDE ANTIGEN AT 2.8 ANGSTROMS  
Authors : Stanfield, R.L.; Wilson, I.A.  
Deposited on : 1991-03-21  
Resolution : 2.80 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](mailto: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.

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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)  
Xtrriage (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

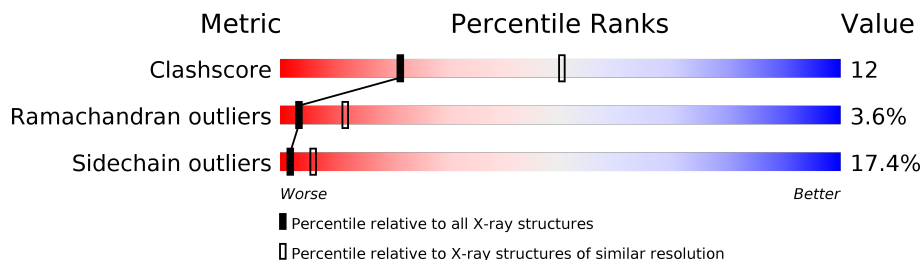
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	219	
1	M	219	
2	H	221	
2	J	221	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6700 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 IGG1-KAPPA B13I2 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1697	1061	284	345	7	0	0	0
1	M	219	1697	1061	284	345	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	ASN	SER	conflict	PIR PC4203
L	27A	THR	SER	conflict	PIR PC4203
L	27C	LEU	VAL	conflict	PIR PC4203
L	27D	LEU	HIS	conflict	PIR PC4203
L	27E	SER	THR	conflict	PIR PC4203
L	28	ASP	ASN	conflict	PIR PC4203
L	30	ASP	ASN	conflict	PIR PC4203
L	96	PRO	ARG	conflict	PIR PC4203
M	26	ASN	SER	conflict	PIR PC4203
M	27A	THR	SER	conflict	PIR PC4203
M	27C	LEU	VAL	conflict	PIR PC4203
M	27D	LEU	HIS	conflict	PIR PC4203
M	27E	SER	THR	conflict	PIR PC4203
M	28	ASP	ASN	conflict	PIR PC4203
M	30	ASP	ASN	conflict	PIR PC4203
M	96	PRO	ARG	conflict	PIR PC4203

- Molecule 2 is a protein called IGG1-KAPPA B13I2 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1646	1040	274	324	8	0	0	0
2	J	218	1646	1040	274	324	8	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

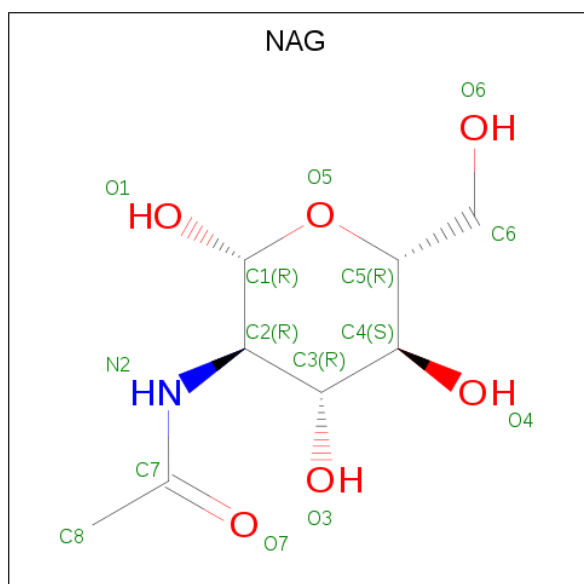
Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	conflict	PIR S38864
H	5	VAL	LEU	conflict	PIR S38864
H	27	PHE	LEU	conflict	PIR S38864
H	31	ARG	SER	conflict	PIR S38864
H	32	CYS	TYR	conflict	PIR S38864
H	33	ALA	GLY	conflict	PIR S38864
H	40	THR	ILE	conflict	PIR S38864
H	42	GLU	ASP	conflict	PIR S38864
H	50	GLY	THR	conflict	PIR S38864
H	55	SER	THR	conflict	PIR S38864
H	58	PHE	TYR	conflict	PIR S38864
H	62	THR	SER	conflict	PIR S38864
H	68	ILE	THR	conflict	PIR S38864
H	72	ASN	ASP	conflict	PIR S38864
H	75	ARG	LYS	conflict	PIR S38864
H	79	SER	TYR	conflict	PIR S38864
H	83	ARG	LYS	conflict	PIR S38864
H	89	ILE	MET	conflict	PIR S38864
H	93	THR	ALA	conflict	PIR S38864
H	?	-	GLN	deletion	PIR S38864
H	95	TYR	GLY	conflict	PIR S38864
H	96	SER	VAL	conflict	PIR S38864
H	98	ASP	THR	conflict	PIR S38864
H	99	PRO	MET	conflict	PIR S38864
H	100	PHE	ILE	conflict	PIR S38864
H	100B	TYR	ARG	conflict	PIR S38864
H	101	ASP	ALA	conflict	PIR S38864
H	108	THR	LEU	conflict	PIR S38864
H	109	LEU	VAL	conflict	PIR S38864
H	113	SER	ALA	conflict	PIR S38864
H	114	ALA	GLY	conflict	PIR S38864
H	198	PRO	THR	conflict	PIR S38864
H	199	ARG	TRP	conflict	PIR S38864
J	3	GLN	LYS	conflict	PIR S38864
J	5	VAL	LEU	conflict	PIR S38864
J	27	PHE	LEU	conflict	PIR S38864
J	31	ARG	SER	conflict	PIR S38864
J	32	CYS	TYR	conflict	PIR S38864
J	33	ALA	GLY	conflict	PIR S38864
J	40	THR	ILE	conflict	PIR S38864
J	42	GLU	ASP	conflict	PIR S38864
J	50	GLY	THR	conflict	PIR S38864

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Chain	Residue	Modelled	Actual	Comment	Reference
J	55	SER	THR	conflict	PIR S38864
J	58	PHE	TYR	conflict	PIR S38864
J	62	THR	SER	conflict	PIR S38864
J	68	ILE	THR	conflict	PIR S38864
J	72	ASN	ASP	conflict	PIR S38864
J	75	ARG	LYS	conflict	PIR S38864
J	79	SER	TYR	conflict	PIR S38864
J	83	ARG	LYS	conflict	PIR S38864
J	89	ILE	MET	conflict	PIR S38864
J	93	THR	ALA	conflict	PIR S38864
J	?	-	GLN	deletion	PIR S38864
J	95	TYR	GLY	conflict	PIR S38864
J	96	SER	VAL	conflict	PIR S38864
J	98	ASP	THR	conflict	PIR S38864
J	99	PRO	MET	conflict	PIR S38864
J	100	PHE	ILE	conflict	PIR S38864
J	100B	TYR	ARG	conflict	PIR S38864
J	101	ASP	ALA	conflict	PIR S38864
J	108	THR	LEU	conflict	PIR S38864
J	109	LEU	VAL	conflict	PIR S38864
J	113	SER	ALA	conflict	PIR S38864
J	114	ALA	GLY	conflict	PIR S38864
J	198	PRO	THR	conflict	PIR S38864
J	199	ARG	TRP	conflict	PIR S38864

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



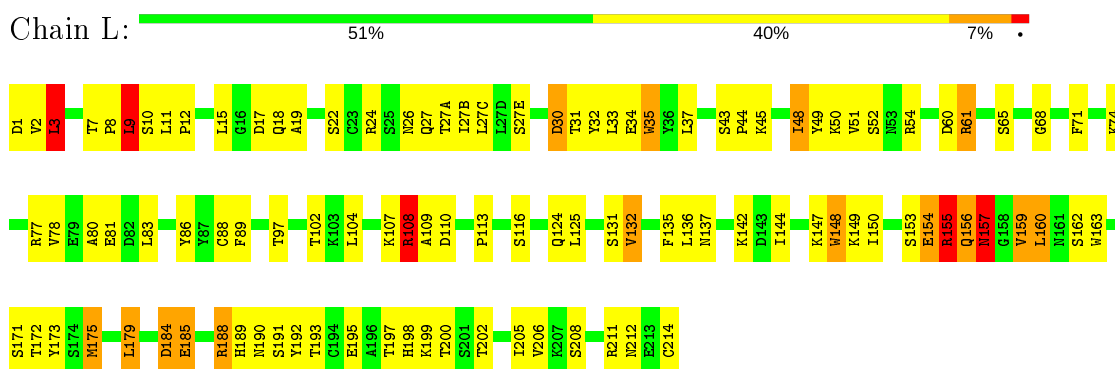
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	L	1	14	8	1	5	0	0

### 3 Residue-property plots

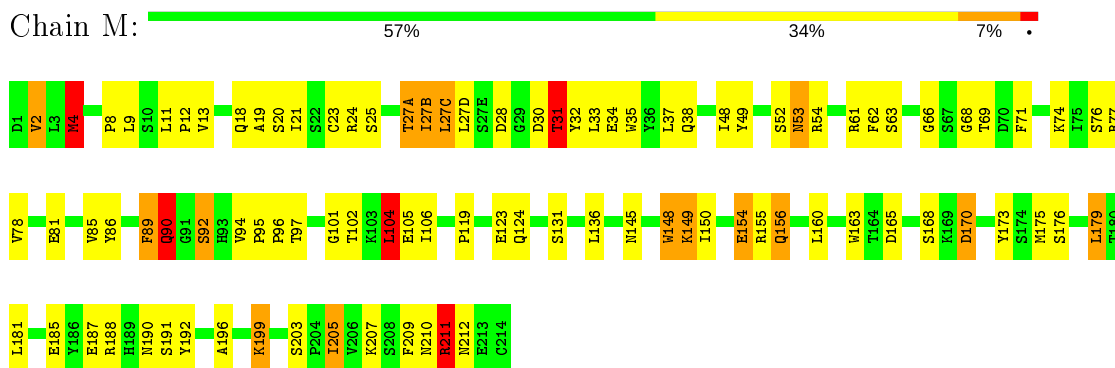
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

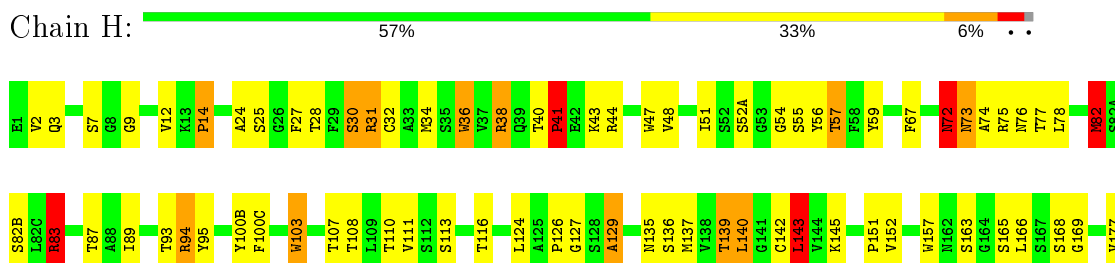
- Molecule 1: IGG1-KAPPA B13I2 FAB (LIGHT CHAIN)



- Molecule 1: IGG1-KAPPA B13I2 FAB (LIGHT CHAIN)



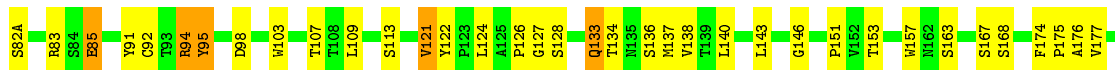
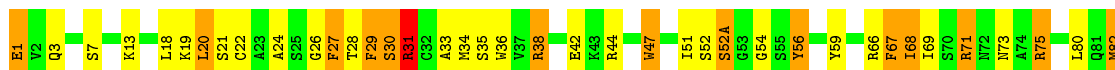
- Molecule 2: IGG1-KAPPA B13I2 FAB (HEAVY CHAIN)





● Molecule 2: IGG1-KAPPA B13I2 FAB (HEAVY CHAIN)

Chain J: 57% 32% 9%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.00 Å 151.70 Å 80.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.95	0/1735	1.74	27/2354 (1.1%)
1	M	0.86	0/1735	1.70	30/2354 (1.3%)
2	H	0.94	2/1689 (0.1%)	1.87	47/2307 (2.0%)
2	J	0.91	0/1689	1.80	40/2307 (1.7%)
All	All	0.91	2/6848 (0.0%)	1.78	144/9322 (1.5%)

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	L	0	1
1	M	0	1
2	H	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	82(B)	SER	CA-CB	5.84	1.61	1.52
2	H	168	SER	CA-CB	5.03	1.60	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	199	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	L	188	ARG	NE-CZ-NH2	-10.82	114.89	120.30
2	H	94	ARG	NE-CZ-NH1	10.74	125.67	120.30
2	J	66	ARG	NE-CZ-NH2	-10.41	115.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	137	MET	CG-SD-CE	-10.35	83.65	100.20
1	M	4	MET	CG-SD-CE	-10.10	84.05	100.20
2	H	82	MET	CG-SD-CE	-9.56	84.91	100.20
2	J	199	ARG	NE-CZ-NH1	9.48	125.04	120.30
2	H	34	MET	CG-SD-CE	-9.46	85.06	100.20
2	J	157	TRP	CD1-CG-CD2	9.18	113.64	106.30
1	M	188	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	M	35	TRP	CD1-CG-CD2	8.99	113.49	106.30
2	J	47	TRP	CD1-CG-CD2	8.84	113.37	106.30
2	J	187	LEU	CA-CB-CG	8.83	135.62	115.30
1	M	163	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	L	148	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	L	104	LEU	CA-CB-CG	8.36	134.52	115.30
2	H	157	TRP	CD1-CG-CD2	8.23	112.89	106.30
2	H	38	ARG	NE-CZ-NH1	8.23	124.41	120.30
2	H	36	TRP	CD1-CG-CD2	8.20	112.86	106.30
2	J	103	TRP	CD1-CG-CD2	7.92	112.63	106.30
2	J	94	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	L	108	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	M	211	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	M	32	TYR	CB-CG-CD2	-7.69	116.39	121.00
1	M	163	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	L	155	ARG	N-CA-C	-7.56	90.58	111.00
1	L	192	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	M	35	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	M	148	TRP	CD1-CG-CD2	7.47	112.28	106.30
2	J	157	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	M	61	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	L	163	TRP	CD1-CG-CD2	7.41	112.23	106.30
2	H	56	TYR	CB-CG-CD2	-7.41	116.56	121.00
2	H	95	TYR	CB-CG-CD1	-7.40	116.56	121.00
2	J	47	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	L	148	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	L	157	ASN	CA-CB-CG	-7.33	97.27	113.40
2	H	103	TRP	CD1-CG-CD2	7.30	112.14	106.30
2	J	36	TRP	CG-CD2-CE3	7.20	140.38	133.90
2	H	36	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	L	35	TRP	CD1-CG-CD2	7.12	112.00	106.30
2	H	47	TRP	CD1-CG-CD2	7.06	111.95	106.30
2	J	31	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	L	83	LEU	CA-CB-CG	7.04	131.49	115.30
1	L	175	MET	CG-SD-CE	-7.03	88.95	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	9	LEU	CA-CB-CG	7.02	131.44	115.30
2	J	103	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	M	148	TRP	CE2-CD2-CG	-6.96	101.73	107.30
2	J	91	TYR	CB-CG-CD2	-6.86	116.89	121.00
2	J	36	TRP	CE2-CD2-CG	-6.83	101.84	107.30
2	J	36	TRP	CD1-CG-CD2	6.83	111.76	106.30
1	L	35	TRP	CE2-CD2-CG	-6.81	101.85	107.30
2	J	20	LEU	CB-CG-CD2	-6.75	99.52	111.00
2	J	122	TYR	CB-CG-CD2	-6.74	116.96	121.00
2	H	157	TRP	CE2-CD2-CG	-6.71	101.93	107.30
2	H	75	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	H	192	THR	CA-CB-CG2	6.62	121.67	112.40
1	L	163	TRP	CE2-CD2-CG	-6.57	102.04	107.30
2	H	47	TRP	CE2-CD2-CG	-6.57	102.05	107.30
1	L	3	LEU	CA-CB-CG	6.44	130.11	115.30
1	M	90	GLN	CA-CB-CG	6.43	127.54	113.40
2	H	137	MET	CA-CB-CG	-6.42	102.39	113.30
2	J	36	TRP	CB-CG-CD1	-6.41	118.67	127.00
2	H	192	THR	CA-CB-OG1	-6.40	95.57	109.00
2	J	31	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	H	103	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	L	159	VAL	CG1-CB-CG2	-6.26	100.88	110.90
2	J	34	MET	CG-SD-CE	-6.21	90.26	100.20
2	H	94	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	J	67	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	M	77	ARG	N-CA-C	-6.04	94.70	111.00
2	J	47	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	M	31	THR	N-CA-C	6.03	127.28	111.00
1	L	1	ASP	N-CA-C	-5.99	94.83	111.00
2	H	44	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	H	183	ASP	CA-CB-CG	5.97	126.53	113.40
2	H	143	LEU	CA-CB-CG	5.91	128.90	115.30
2	H	41	PRO	CA-C-N	5.85	130.06	117.20
1	M	205	ILE	N-CA-C	-5.79	95.37	111.00
2	H	199	ARG	CB-CG-CD	5.78	126.64	111.60
1	M	35	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	M	104	LEU	CA-CB-CG	5.76	128.55	115.30
1	M	211	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	J	20	LEU	CA-CB-CG	5.72	128.46	115.30
2	J	157	TRP	CG-CD1-NE1	-5.66	104.44	110.10
2	H	2	VAL	N-CA-C	-5.65	95.75	111.00
1	M	136	LEU	CA-CB-CG	5.62	128.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	134	THR	N-CA-C	-5.60	95.88	111.00
2	H	47	TRP	CG-CD2-CE3	5.54	138.89	133.90
2	H	31	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	J	75	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	M	179	LEU	CA-CB-CG	5.51	127.97	115.30
2	H	14	PRO	N-CA-C	5.50	126.41	112.10
2	H	32	CYS	N-CA-CB	-5.50	100.70	110.60
2	J	44	ARG	CA-CB-CG	5.49	125.47	113.40
1	M	185	GLU	CA-CB-CG	5.47	125.44	113.40
2	J	200	PRO	N-CD-CG	-5.45	95.02	103.20
1	M	27(A)	THR	CA-C-N	-5.45	105.21	117.20
1	M	106	ILE	CB-CG1-CD1	-5.44	98.66	113.90
1	L	163	TRP	CE2-CD2-CE3	5.42	125.20	118.70
2	H	83	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	H	36	TRP	CG-CD1-NE1	-5.39	104.71	110.10
2	H	157	TRP	CG-CD1-NE1	-5.39	104.71	110.10
2	J	66	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	L	60	ASP	CA-C-N	-5.38	105.37	117.20
2	H	185	TYR	CB-CG-CD1	-5.37	117.78	121.00
2	H	38	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	M	188	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	J	82	MET	CG-SD-CE	-5.35	91.65	100.20
2	H	178	LEU	CA-CB-CG	5.34	127.57	115.30
1	L	156	GLN	CA-CB-CG	-5.33	101.67	113.40
1	M	163	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	M	173	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	M	123	GLU	CB-CG-CD	5.25	128.37	114.20
1	L	157	ASN	C-N-CA	5.24	133.30	122.30
2	H	100(B)	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	L	54	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	J	103	TRP	CG-CD1-NE1	-5.22	104.88	110.10
2	H	78	LEU	O-C-N	-5.21	114.37	122.70
2	J	52(A)	SER	N-CA-C	5.21	125.06	111.00
1	L	107	LYS	CA-C-N	-5.21	105.75	117.20
2	H	129	ALA	N-CA-CB	5.19	117.36	110.10
2	J	38	ARG	CD-NE-CZ	-5.18	116.34	123.60
2	J	30	SER	N-CA-CB	-5.18	102.73	110.50
2	J	44	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	H	59	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	J	71	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	M	154	GLU	CA-C-N	-5.11	105.95	117.20
2	H	57	THR	CA-CB-OG1	-5.11	98.28	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	27(C)	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	H	57	THR	CA-CB-CG2	5.09	119.53	112.40
2	H	187	LEU	CA-CB-CG	5.09	127.01	115.30
1	M	192	TYR	CB-CG-CD1	-5.09	117.95	121.00
2	J	20	LEU	CB-CG-CD1	5.08	119.64	111.00
2	J	85	GLU	CA-CB-CG	5.08	124.58	113.40
2	J	47	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	L	61	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	M	76	SER	N-CA-C	5.06	124.66	111.00
2	H	103	TRP	CG-CD1-NE1	-5.05	105.05	110.10
2	H	127	GLY	N-CA-C	-5.04	100.51	113.10
2	J	29	PHE	CA-C-N	-5.02	106.15	117.20
1	L	30	ASP	C-N-CA	5.01	134.23	121.70
2	H	94	ARG	CB-CG-CD	-5.01	98.58	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	40	THR	Peptide
1	L	154	GLU	Mainchain
1	M	94	VAL	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	1697	0	1638	51	0
1	M	1697	0	1639	42	0
2	H	1646	0	1614	31	0
2	J	1646	0	1614	41	0
3	L	14	0	13	0	0
All	All	6700	0	6518	158	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 12.

All (158) 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:199:ARG:HB3	2:H:199:ARG:HH11	1.27	0.98
2:H:89:ILE:HG12	2:H:108:THR:HG22	1.47	0.97
1:L:150:ILE:HB	1:L:154:GLU:HB2	1.67	0.77
1:L:27(B):ILE:HG22	1:L:31:THR:HG23	1.69	0.73
2:H:72:ASN:HB3	2:H:77:THR:HB	1.71	0.71
2:H:199:ARG:HD2	2:H:199:ARG:O	1.91	0.71
1:M:190:ASN:HA	1:M:211:ARG:HB2	1.73	0.70
2:J:163:SER:H	2:J:209:ASN:HD21	1.37	0.70
2:H:87:THR:HG23	2:H:110:THR:HA	1.73	0.69
1:M:34:GLU:HG3	1:M:49:TYR:HA	1.77	0.67
2:H:196:SER:HB2	2:H:198:PRO:HD3	1.79	0.64
2:J:209:ASN:HB3	2:J:218:LYS:NZ	2.11	0.64
2:J:199:ARG:HG3	2:J:200:PRO:HG3	1.80	0.62
2:J:194:PRO:O	2:J:198:PRO:HD2	1.99	0.62
1:M:25:SER:HB2	1:M:27(B):ILE:HD11	1.82	0.61
1:M:31:THR:HG21	1:M:71:PHE:CZ	2.36	0.61
2:J:51:ILE:HD11	2:J:54:GLY:HA2	1.82	0.61
2:H:30:SER:O	2:H:52(A):SER:HB3	2.01	0.61
2:J:59:TYR:OH	2:J:69:ILE:HG22	2.01	0.60
2:H:199:ARG:HH11	2:H:199:ARG:CB	2.09	0.60
1:M:119:PRO:HB3	1:M:209:PHE:CE2	2.37	0.59
1:M:27(C):LEU:CB	1:M:68:GLY:HA2	2.32	0.59
1:L:149:LYS:HA	1:L:154:GLU:O	2.01	0.59
2:J:24:ALA:HB1	2:J:27:PHE:HE1	1.68	0.58
2:J:138:VAL:HG21	2:J:199:ARG:HB2	1.84	0.58
1:L:160:LEU:HG	2:H:177:VAL:HG21	1.86	0.58
1:L:155:ARG:NH1	2:J:146:GLY:HA3	2.19	0.58
2:H:169:GLY:O	2:H:191:VAL:HA	2.03	0.57
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.39	0.57
1:M:21:ILE:HG12	1:M:102:THR:HG21	1.86	0.57
1:L:147:LYS:HG2	1:L:195:GLU:HB3	1.87	0.57
2:J:199:ARG:O	2:J:199:ARG:NH1	2.38	0.56
2:H:9:GLY:HA3	2:H:108:THR:O	2.06	0.56
1:L:33:LEU:HD22	1:L:89:PHE:O	2.05	0.56
1:L:208:SER:O	2:H:129:ALA:HB2	2.05	0.56
1:L:108:ARG:HG2	1:L:171:SER:HB2	1.88	0.55
2:H:194:PRO:HB2	2:H:198:PRO:HD2	1.89	0.55
1:L:9:LEU:H	1:L:9:LEU:HD13	1.70	0.55
2:J:199:ARG:HB3	2:J:200:PRO:HD3	1.89	0.54
1:M:49:TYR:CE1	1:M:53:ASN:HB2	2.42	0.54
2:H:194:PRO:O	2:H:198:PRO:HD2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:96:PRO:HD2	2:J:47:TRP:CE3	2.42	0.54
1:L:142:LYS:HB2	1:L:173:TYR:CE1	2.42	0.54
1:M:85:VAL:HA	1:M:102:THR:O	2.06	0.54
2:J:30:SER:O	2:J:31:ARG:HG2	2.08	0.54
2:J:19:LYS:HA	2:J:80:LEU:O	2.07	0.53
2:H:12:VAL:O	2:H:111:VAL:HA	2.08	0.53
1:L:132:VAL:HG13	1:L:179:LEU:HB3	1.88	0.53
1:M:86:TYR:O	1:M:101:GLY:HA2	2.08	0.53
1:L:3:LEU:HD12	1:L:26:ASN:HB3	1.91	0.53
1:M:27(B):ILE:HD12	1:M:71:PHE:HE2	1.73	0.52
2:J:199:ARG:HH21	2:J:227:PRO:HD3	1.74	0.52
1:M:4:MET:CE	1:M:90:GLN:HB2	2.39	0.52
2:J:35:SER:HB2	2:J:95:TYR:CE2	2.45	0.52
1:L:148:TRP:CE3	1:L:179:LEU:HD12	2.44	0.52
2:H:199:ARG:NH1	2:H:199:ARG:HB3	2.10	0.52
1:M:27(C):LEU:HB2	1:M:68:GLY:HA2	1.92	0.52
2:H:93:THR:CG2	2:H:100(C):PHE:HB3	2.40	0.51
2:J:13:LYS:HD3	2:J:113:SER:HA	1.92	0.51
2:J:59:TYR:OH	2:J:68:ILE:HA	2.12	0.50
1:M:48:ILE:HG23	1:M:52:SER:HA	1.93	0.50
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.94	0.50
2:J:174:PHE:O	2:J:187:LEU:HD22	2.12	0.50
1:L:149:LYS:HB2	1:L:193:THR:HB	1.94	0.50
1:M:27(B):ILE:HD12	1:M:71:PHE:CE2	2.46	0.50
1:M:11:LEU:HD21	1:M:19:ALA:HB1	1.93	0.50
2:J:140:LEU:HD21	2:J:199:ARG:HD2	1.95	0.49
2:J:1:GLU:O	2:J:26:GLY:HA3	2.12	0.49
1:L:37:LEU:HD13	1:L:86:TYR:CZ	2.47	0.49
1:M:4:MET:SD	1:M:90:GLN:HB2	2.53	0.49
1:L:136:LEU:HD23	1:L:144:ILE:HD11	1.95	0.49
1:M:11:LEU:HD23	1:M:104:LEU:HD22	1.92	0.49
1:M:149:LYS:HA	1:M:154:GLU:O	2.13	0.49
1:M:13:VAL:HG21	1:M:78:VAL:HG21	1.95	0.49
1:L:8:PRO:O	1:L:102:THR:HG23	2.13	0.48
1:M:148:TRP:O	1:M:155:ARG:HA	2.12	0.48
1:L:185:GLU:OE1	1:L:189:HIS:HE1	1.96	0.48
1:M:27(C):LEU:HB3	1:M:68:GLY:HA2	1.94	0.48
1:L:156:GLN:HG2	1:L:157:ASN:N	2.29	0.47
1:L:184:ASP:O	1:L:188:ARG:HG3	2.15	0.47
1:M:8:PRO:HG2	1:M:11:LEU:HD13	1.95	0.47
2:J:24:ALA:HB1	2:J:27:PHE:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:27:PHE:CE2	2:J:94:ARG:HD2	2.50	0.47
1:M:2:VAL:O	1:M:97:THR:HG21	2.15	0.47
2:H:143:LEU:HD13	2:H:145:LYS:HB2	1.96	0.47
2:H:140:LEU:HD11	2:H:199:ARG:HG3	1.97	0.46
1:L:124:GLN:HE22	1:L:131:SER:H	1.62	0.46
2:J:33:ALA:O	2:J:95:TYR:HB2	2.15	0.46
1:M:150:ILE:HA	1:M:191:SER:O	2.16	0.46
2:H:36:TRP:O	2:H:48:VAL:HG12	2.16	0.46
2:J:153:THR:OG1	2:J:211:ALA:HB3	2.15	0.46
2:J:121:VAL:HA	2:J:143:LEU:O	2.15	0.46
1:L:124:GLN:NE2	1:L:131:SER:H	2.14	0.46
1:M:27(D):LEU:HD22	1:M:92:SER:HB3	1.98	0.46
2:J:67:PHE:CD1	2:J:82:MET:HA	2.51	0.45
1:L:9:LEU:H	1:L:9:LEU:CD1	2.30	0.45
2:H:140:LEU:HD22	2:H:140:LEU:N	2.31	0.45
2:J:176:ALA:HA	2:J:186:THR:O	2.16	0.45
1:M:12:PRO:HA	1:M:105:GLU:O	2.17	0.45
1:M:196:ALA:HB3	1:M:205:ILE:HB	1.98	0.45
2:J:30:SER:HB3	2:J:73:ASN:HD22	1.82	0.45
1:M:66:GLY:HA3	1:M:71:PHE:HA	1.99	0.45
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.51	0.45
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.82	0.45
1:L:34:GLU:HG3	1:L:49:TYR:HA	1.98	0.45
2:H:72:ASN:O	2:H:74:ALA:N	2.50	0.44
1:L:144:ILE:HG13	1:L:198:HIS:HB2	1.99	0.44
2:J:33:ALA:HA	2:J:71:ARG:NH2	2.33	0.44
1:L:33:LEU:HG	1:L:71:PHE:CG	2.53	0.44
1:M:160:LEU:HG	2:J:177:VAL:HG11	1.99	0.44
1:L:148:TRP:O	1:L:155:ARG:HA	2.17	0.44
1:M:37:LEU:HD12	1:M:38:GLN:N	2.32	0.44
1:L:35:TRP:HD1	1:L:48:ILE:CG2	2.31	0.43
2:J:52:SER:HG	2:J:56:TYR:HD1	1.64	0.43
2:J:80:LEU:HA	2:J:80:LEU:HD23	1.83	0.43
2:J:38:ARG:HD3	2:J:38:ARG:HH11	1.63	0.43
2:J:215:SER:O	2:J:217:THR:N	2.51	0.43
1:L:22:SER:HB2	1:L:24:ARG:HH12	1.84	0.43
2:J:126:PRO:HG3	2:J:199:ARG:HD3	2.00	0.43
2:J:163:SER:N	2:J:209:ASN:HD21	2.12	0.42
1:L:195:GLU:HG3	1:L:206:VAL:HG22	2.01	0.42
2:J:209:ASN:HB3	2:J:218:LYS:HZ3	1.84	0.42
1:M:54:ARG:HD3	1:M:62:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:153:SER:O	1:L:155:ARG:N	2.52	0.42
2:H:139:THR:HB	2:H:192:THR:OG1	2.18	0.42
1:M:207:LYS:HZ2	2:J:128:SER:HB3	1.84	0.42
1:L:7:THR:OG1	1:L:24:ARG:NH2	2.52	0.42
2:H:67:PHE:CD1	2:H:82:MET:HB3	2.54	0.42
1:L:190:ASN:HA	1:L:211:ARG:HG2	2.01	0.42
1:L:9:LEU:HD22	1:L:10:SER:N	2.35	0.42
2:H:83:ARG:HG2	2:H:83:ARG:H	1.55	0.41
1:L:162:SER:O	1:L:175:MET:HA	2.20	0.41
1:L:32:TYR:CD2	1:L:50:LYS:HD3	2.55	0.41
1:M:31:THR:HG22	1:M:33:LEU:HB2	2.02	0.41
1:L:113:PRO:HG2	1:L:205:ILE:HD12	2.02	0.41
1:M:89:PHE:HA	1:M:97:THR:O	2.20	0.41
1:L:17:ASP:O	1:L:78:VAL:HG23	2.19	0.41
1:L:2:VAL:HG13	1:L:27:GLN:HB3	2.03	0.41
1:L:44:PRO:HD2	2:H:103:TRP:CE3	2.55	0.41
2:J:138:VAL:CG2	2:J:199:ARG:HB2	2.51	0.41
2:J:199:ARG:CB	2:J:200:PRO:HD3	2.50	0.41
1:M:19:ALA:O	1:M:74:LYS:HA	2.21	0.41
2:H:126:PRO:HD3	2:H:140:LEU:HD12	2.03	0.41
1:M:124:GLN:HE22	1:M:131:SER:HB2	1.86	0.41
1:M:95:PRO:HA	1:M:96:PRO:HD3	1.94	0.41
1:L:9:LEU:HD22	1:L:10:SER:H	1.86	0.41
1:L:19:ALA:O	1:L:74:LYS:HA	2.21	0.41
2:H:143:LEU:CD1	2:H:145:LYS:HD2	2.51	0.40
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.56	0.40
1:L:11:LEU:HA	1:L:12:PRO:HD3	1.88	0.40
1:L:108:ARG:HD3	1:L:109:ALA:O	2.20	0.40
1:L:15:LEU:HD21	1:L:80:ALA:HA	2.03	0.40
1:L:125:LEU:HA	1:L:125:LEU:HD12	1.78	0.40
1:M:150:ILE:HD13	1:M:156:GLN:HG3	2.03	0.40
1:L:110:ASP:HB3	1:L:200:THR:HG22	2.04	0.40
1:L:150:ILE:HB	1:L:154:GLU:CB	2.46	0.40
1:M:27(C):LEU:HA	1:M:31:THR:OG1	2.21	0.40
1:M:175:MET:HG2	1:M:176:SER:N	2.36	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	217/219 (99%)	196 (90%)	16 (7%)	5 (2%)	6	21
1	M	217/219 (99%)	195 (90%)	15 (7%)	7 (3%)	4	13
2	H	216/221 (98%)	186 (86%)	20 (9%)	10 (5%)	2	7
2	J	216/221 (98%)	185 (86%)	22 (10%)	9 (4%)	3	9
All	All	866/880 (98%)	762 (88%)	73 (8%)	31 (4%)	3	11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	61	ARG
1	L	212	ASN
2	H	41	PRO
2	H	73	ASN
1	M	30	ASP
2	J	52(A)	SER
2	J	168	SER
1	L	51	VAL
1	L	68	GLY
1	L	199	LYS
2	H	43	LYS
2	H	136	SER
2	H	214	ALA
1	M	170	ASP
2	J	31	ARG
2	J	136	SER
2	J	216	SER
2	H	198	PRO
1	M	168	SER
1	M	199	LYS
1	M	211	ARG
2	H	14	PRO

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Mol	Chain	Res	Type
2	H	72	ASN
2	H	163	SER
1	M	31	THR
2	J	133	GLN
2	J	200	PRO
2	J	214	ALA
1	M	81	GLU
2	H	200	PRO
2	J	127	GLY

### 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	196/196 (100%)	167 (85%)	29 (15%)	3	9
1	M	196/196 (100%)	165 (84%)	31 (16%)	2	8
2	H	189/192 (98%)	151 (80%)	38 (20%)	1	4
2	J	189/192 (98%)	153 (81%)	36 (19%)	1	4
All	All	770/776 (99%)	636 (83%)	134 (17%)	2	6

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	LEU
1	L	9	LEU
1	L	18	GLN
1	L	27(A)	THR
1	L	27(E)	SER
1	L	30	ASP
1	L	43	SER
1	L	45	LYS
1	L	48	ILE
1	L	52	SER
1	L	65	SER
1	L	77	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	81	GLU
1	L	97	THR
1	L	108	ARG
1	L	116	SER
1	L	132	VAL
1	L	155	ARG
1	L	157	ASN
1	L	159	VAL
1	L	160	LEU
1	L	172	THR
1	L	179	LEU
1	L	184	ASP
1	L	185	GLU
1	L	191	SER
1	L	197	THR
1	L	202	THR
1	L	214	CYS
2	H	3	GLN
2	H	7	SER
2	H	25	SER
2	H	28	THR
2	H	30	SER
2	H	31	ARG
2	H	38	ARG
2	H	41	PRO
2	H	55	SER
2	H	57	THR
2	H	72	ASN
2	H	73	ASN
2	H	76	ASN
2	H	82	MET
2	H	83	ARG
2	H	94	ARG
2	H	107	THR
2	H	113	SER
2	H	116	THR
2	H	124	LEU
2	H	135	ASN
2	H	139	THR
2	H	140	LEU
2	H	142	CYS
2	H	143	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	151	PRO
2	H	152	VAL
2	H	165	SER
2	H	166	LEU
2	H	180	SER
2	H	184	LEU
2	H	192	THR
2	H	196	SER
2	H	199	ARG
2	H	204	THR
2	H	208	CYS
2	H	216	SER
2	H	217	THR
1	M	2	VAL
1	M	4	MET
1	M	9	LEU
1	M	18	GLN
1	M	20	SER
1	M	23	CYS
1	M	24	ARG
1	M	27(A)	THR
1	M	27(B)	ILE
1	M	27(C)	LEU
1	M	28	ASP
1	M	53	ASN
1	M	63	SER
1	M	69	THR
1	M	89	PHE
1	M	90	GLN
1	M	92	SER
1	M	104	LEU
1	M	145	ASN
1	M	149	LYS
1	M	156	GLN
1	M	165	ASP
1	M	170	ASP
1	M	179	LEU
1	M	181	LEU
1	M	187	GLU
1	M	199	LYS
1	M	203	SER
1	M	210	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	211	ARG
1	M	212	ASN
2	J	1	GLU
2	J	3	GLN
2	J	7	SER
2	J	18	LEU
2	J	20	LEU
2	J	21	SER
2	J	22	CYS
2	J	27	PHE
2	J	28	THR
2	J	29	PHE
2	J	31	ARG
2	J	42	GLU
2	J	56	TYR
2	J	68	ILE
2	J	75	ARG
2	J	82(A)	SER
2	J	83	ARG
2	J	85	GLU
2	J	92	CYS
2	J	95	TYR
2	J	98	ASP
2	J	107	THR
2	J	109	LEU
2	J	121	VAL
2	J	124	LEU
2	J	133	GLN
2	J	137	MET
2	J	151	PRO
2	J	167	SER
2	J	175	PRO
2	J	183	ASP
2	J	184	LEU
2	J	187	LEU
2	J	196	SER
2	J	199	ARG
2	J	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	124	GLN
1	L	137	ASN
1	L	161	ASN
2	H	3	GLN
1	M	124	GLN
1	M	190	ASN
1	M	210	ASN
2	J	76	ASN
2	J	135	ASN
2	J	179	GLN
2	J	209	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	$\# Z  > 2$
3	NAG	L	901	1	14,14,15	0.73	0	17,19,21	1.62	2 (11%)



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	NAG	L	901	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	901	NAG	O5-C1-C2	-4.56	104.08	111.29
3	L	901	NAG	C1-O5-C5	3.82	117.37	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	901	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 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

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.