



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:35 AM UTC

PDB ID : 1IGF / pdb_00001igf
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.

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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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

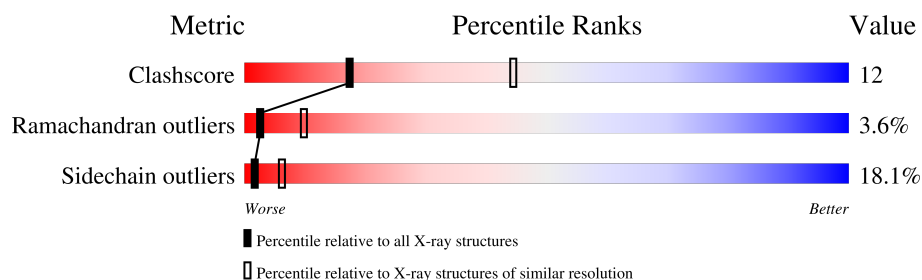
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

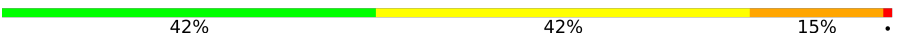
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	219	 42% 42% 15% .
1	M	219	 54% 36% 6% .
2	H	221	 48% 37% 10% . .
2	J	221	 52% 34% 11% ..

2 Entry composition

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
1	L	219	Total	C	N	O	S	0	0	0
			1697	1061	284	345	7			
1	M	219	Total	C	N	O	S	0	0	0
			1697	1061	284	345	7			

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
2	H	218	Total	C	N	O	S	0	0	0
			1646	1040	274	324	8			
2	J	218	Total	C	N	O	S	0	0	0
			1646	1040	274	324	8			

There are 66 discrepancies between the modelled and reference sequences:

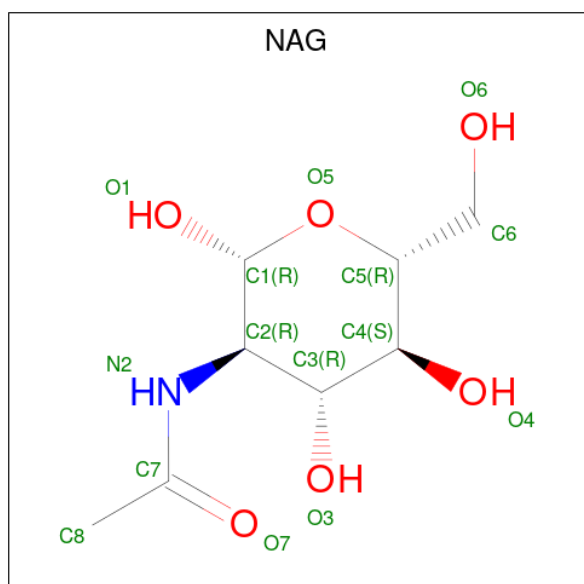
Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	conflict	PIR S38864
H	5	VAL	LEU	conflict	PIR S38864
H	27	PHE	LEU	conflict	PIR S38864
H	31	ARG	SER	conflict	PIR S38864
H	32	CYS	TYR	conflict	PIR S38864
H	33	ALA	GLY	conflict	PIR S38864
H	40	THR	ILE	conflict	PIR S38864
H	42	GLU	ASP	conflict	PIR 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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



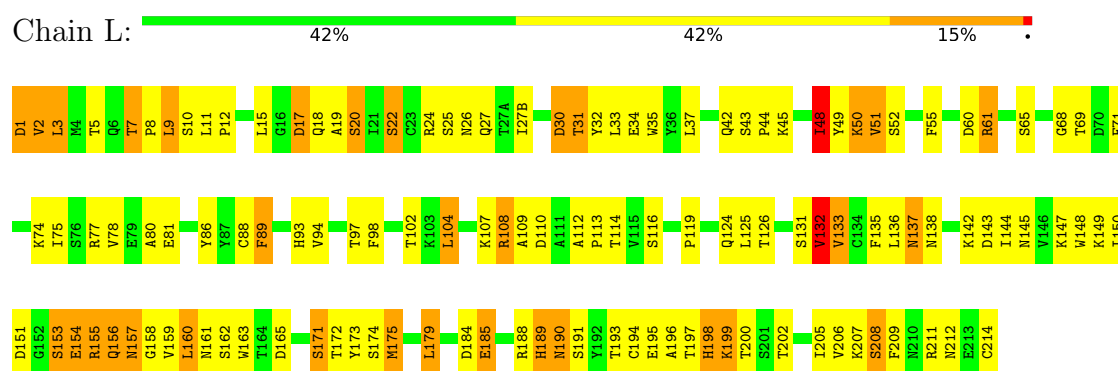
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

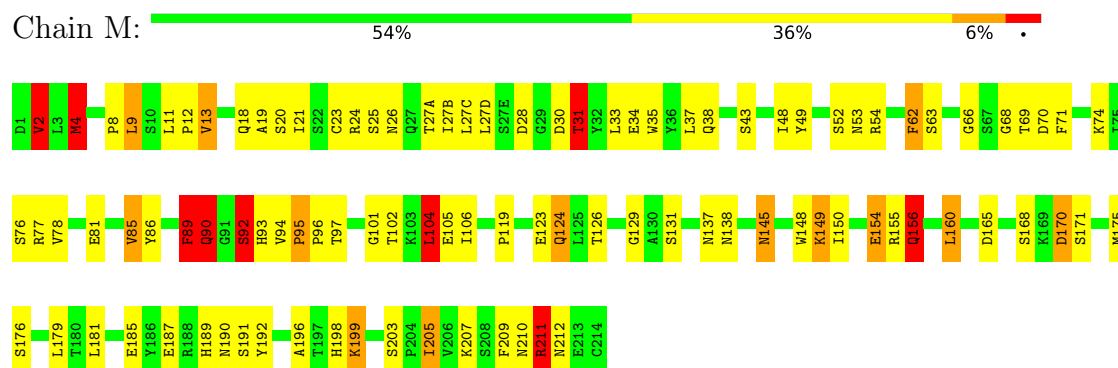
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

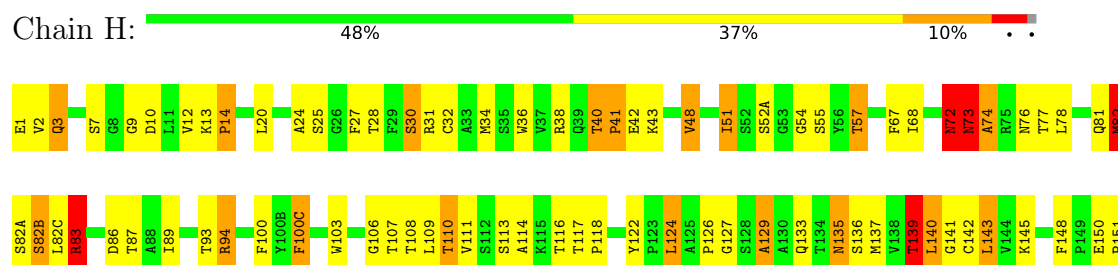
• Molecule 1: IGG1-KAPPA B13I2 FAB (LIGHT CHAIN)



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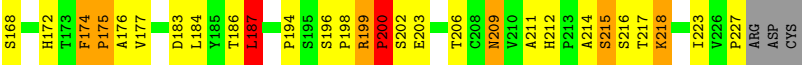
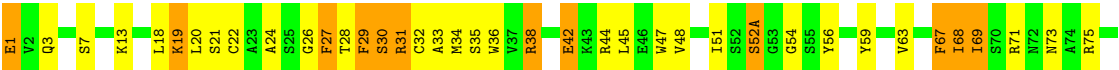


• Molecule 2: IGG1-KAPPA B13I2 FAB (HEAVY CHAIN)





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



4 Data and refinement statistics

Xtriage (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, α , β , γ	98.00Å 151.70Å 80.80Å 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.	Xtriage
Total number of atoms	6700	wwPDB-VP
Average B, all atoms (Å ²)	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	1.20	7/1735 (0.4%)	2.10	63/2354 (2.7%)
1	M	1.07	4/1735 (0.2%)	2.00	47/2354 (2.0%)
2	H	1.14	4/1689 (0.2%)	2.14	74/2307 (3.2%)
2	J	1.10	5/1689 (0.3%)	1.99	45/2307 (2.0%)
All	All	1.13	20/6848 (0.3%)	2.06	229/9322 (2.5%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	212	HIS	CD2-NE2	-7.15	1.29	1.37
1	M	198	HIS	CD2-NE2	-6.92	1.30	1.37
1	M	189	HIS	CD2-NE2	-6.71	1.30	1.37
1	L	189	HIS	CD2-NE2	-6.68	1.30	1.37
1	L	198	HIS	CD2-NE2	-6.59	1.30	1.37
2	J	172	HIS	CD2-NE2	-6.54	1.30	1.37
1	M	93	HIS	CD2-NE2	-6.29	1.30	1.37
1	L	153	SER	CA-C	-6.24	1.45	1.53
2	H	172	HIS	CD2-NE2	-6.22	1.31	1.37
2	J	212	HIS	CD2-NE2	-6.17	1.31	1.37
1	L	133	VAL	CA-CB	6.15	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	93	HIS	CD2-NE2	-6.12	1.31	1.37
2	H	212	HIS	CG-ND1	-5.69	1.31	1.38
1	L	198	HIS	CG-ND1	-5.65	1.32	1.38
2	H	82(B)	SER	CA-CB	5.57	1.61	1.53
1	M	189	HIS	CG-ND1	-5.53	1.32	1.38
2	J	172	HIS	CG-ND1	-5.25	1.32	1.38
2	J	122	TYR	CA-CB	-5.19	1.43	1.54
1	L	158	GLY	CA-C	5.05	1.59	1.51
2	J	212	HIS	CG-ND1	-5.00	1.32	1.38

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	157	ASN	CA-CB-CG	-15.33	97.27	112.60
2	H	183	ASP	CA-CB-CG	13.93	126.53	112.60
1	L	155	ARG	N-CA-C	-11.56	90.58	108.96
2	H	76	ASN	OD1-CG-ND2	-11.27	111.33	122.60
1	M	28	ASP	CA-CB-CG	9.83	122.43	112.60
2	H	192	THR	CA-CB-OG1	-9.36	95.57	109.60
1	M	123	GLU	CB-CG-CD	9.28	128.37	112.60
1	L	60	ASP	CA-CB-CG	9.17	121.77	112.60
1	M	26	ASN	CA-CB-CG	9.17	121.77	112.60
1	L	30	ASP	CA-C-N	8.93	134.23	120.75
1	L	30	ASP	C-N-CA	8.93	134.23	120.75
2	H	10	ASP	CA-CB-CG	8.69	121.28	112.60
2	H	2	VAL	N-CA-C	-8.53	95.75	108.97
2	J	29	PHE	CA-C-O	8.52	129.47	120.70
1	L	31	THR	N-CA-C	8.41	121.79	110.35
1	M	205	ILE	N-CA-C	-8.41	95.37	108.23
2	H	100	PHE	CA-CB-CG	-7.99	105.81	113.80
2	H	137	MET	CG-SD-CE	-7.84	83.65	100.90
1	L	42	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	L	190	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	M	31	THR	N-CA-C	7.74	127.28	110.80
2	H	78	LEU	O-C-N	-7.73	114.37	123.41
1	M	4	MET	CG-SD-CE	-7.66	84.05	100.90
2	H	57	THR	CA-CB-OG1	-7.55	98.28	109.60
2	J	67	PHE	CA-CB-CG	7.53	121.33	113.80
2	H	193	VAL	N-CA-CB	-7.36	100.90	111.21
2	H	72	ASN	CA-CB-CG	7.32	119.92	112.60
2	H	137	MET	N-CA-C	7.30	120.84	109.52
2	H	82	MET	CG-SD-CE	-7.27	84.91	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	135	ASN	CA-CB-CG	7.26	119.86	112.60
2	H	129	ALA	N-CA-C	-7.25	99.25	109.69
2	J	166	LEU	CA-C-O	7.24	128.23	120.63
1	M	106	ILE	CB-CG1-CD1	-7.21	98.66	113.80
1	L	153	SER	N-CA-C	-7.20	100.54	111.56
2	H	34	MET	CG-SD-CE	-7.20	85.06	100.90
1	M	89	PHE	CA-CB-CG	7.19	120.99	113.80
2	J	105	GLN	OE1-CD-NE2	-7.12	115.48	122.60
1	M	62	PHE	CA-CB-CG	-7.11	106.69	113.80
2	H	133	GLN	N-CA-C	7.02	114.54	108.78
2	H	74	ALA	N-CA-C	-6.93	103.34	111.03
2	H	14	PRO	N-CA-C	6.76	126.41	112.47
1	L	157	ASN	N-CA-C	6.76	120.05	108.02
1	M	138	ASN	N-CA-C	6.75	119.46	111.02
1	L	98	PHE	CA-CB-CG	6.74	120.54	113.80
1	M	90	GLN	CA-CB-CG	6.72	127.54	114.10
2	J	52(A)	SER	N-CA-C	6.70	125.06	110.80
2	H	199	ARG	CB-CG-CD	6.67	126.64	111.30
2	H	117	THR	CA-C-N	6.66	124.45	119.66
2	H	117	THR	C-N-CA	6.66	124.45	119.66
2	H	48	VAL	CB-CA-C	6.65	116.88	110.63
2	J	203	GLU	N-CA-C	-6.62	98.60	109.40
2	H	76	ASN	CB-CG-ND2	6.60	126.30	116.40
1	L	112	ALA	CA-C-N	6.58	126.56	119.78
1	L	112	ALA	C-N-CA	6.58	126.56	119.78
2	H	192	THR	CA-CB-CG2	6.57	121.67	110.50
1	M	77	ARG	N-CA-C	-6.56	94.70	107.62
2	J	69	ILE	N-CA-C	6.56	116.16	106.85
2	J	42	GLU	CB-CG-CD	6.52	123.69	112.60
1	M	76	SER	N-CA-C	6.51	124.66	110.80
1	M	198	HIS	CB-CG-CD2	-6.49	122.76	131.20
2	J	36	TRP	CG-CD2-CE3	6.48	140.38	133.90
1	L	138	ASN	CA-CB-CG	6.46	119.06	112.60
1	M	156	GLN	OE1-CD-NE2	-6.44	116.16	122.60
2	J	98	ASP	CA-CB-CG	6.42	119.02	112.60
1	L	163	TRP	CE2-CD2-CE3	6.40	125.20	118.80
1	L	94	VAL	N-CA-C	6.39	115.92	108.96
1	L	209	PHE	CA-CB-CG	6.36	120.16	113.80
1	M	156	GLN	N-CA-C	6.35	117.81	108.86
1	L	171	SER	N-CA-C	6.35	120.34	112.47
1	M	95	PRO	CA-C-N	6.34	126.37	119.90
1	M	95	PRO	C-N-CA	6.34	126.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	29	PHE	N-CA-C	6.31	117.96	111.14
1	L	1	ASP	CA-CB-CG	6.29	118.89	112.60
1	L	93	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	M	211	ARG	N-CA-C	6.25	124.11	110.80
2	J	45	LEU	O-C-N	-6.24	115.89	123.19
1	L	156	GLN	CA-CB-CG	-6.22	101.67	114.10
2	H	209	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	H	148	PHE	O-C-N	-6.21	117.50	121.85
2	H	32	CYS	N-CA-CB	-6.20	100.70	110.69
1	M	93	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	L	165	ASP	N-CA-C	-6.16	101.85	110.35
2	J	215	SER	CA-C-O	-6.16	113.68	120.33
1	L	132	VAL	N-CA-C	-6.15	99.56	108.17
1	L	189	HIS	CB-CG-CD2	-6.13	123.22	131.20
2	J	101	ASP	CA-CB-CG	6.13	118.73	112.60
1	L	208	SER	CA-CB-OG	-6.13	98.85	111.10
1	L	157	ASN	CA-C-N	6.07	133.30	121.41
1	L	157	ASN	C-N-CA	6.07	133.30	121.41
2	H	218	LYS	N-CA-C	-6.06	97.97	108.69
1	L	17	ASP	O-C-N	6.03	129.73	122.68
2	J	133	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	M	26	ASN	N-CA-C	-5.98	105.57	112.92
2	H	100(C)	PHE	O-C-N	-5.97	116.23	123.16
2	H	114	ALA	N-CA-C	5.97	119.14	110.42
1	L	137	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	L	60	ASP	N-CA-C	-5.93	100.60	109.15
2	H	106	GLY	CA-C-O	-5.91	116.69	121.77
2	J	134	THR	N-CA-C	-5.87	95.88	107.69
2	H	137	MET	CA-CB-CG	-5.85	102.39	114.10
2	H	81	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	L	138	ASN	N-CA-C	5.84	117.75	110.91
2	J	215	SER	N-CA-C	-5.83	97.64	108.02
1	M	92	SER	CA-CB-OG	5.82	122.75	111.10
2	J	105	GLN	N-CA-C	5.81	120.09	112.89
1	L	69	THR	CA-CB-OG1	-5.80	100.89	109.60
1	L	1	ASP	N-CA-C	-5.78	94.83	111.00
1	L	89	PHE	CA-CB-CG	5.76	119.56	113.80
1	L	199	LYS	N-CA-C	5.76	123.08	110.80
2	J	38	ARG	CD-NE-CZ	-5.76	116.34	124.40
1	M	137	ASN	OD1-CG-ND2	-5.75	116.85	122.60
2	H	73	ASN	N-CA-C	5.74	123.03	110.80
1	L	145	ASN	CA-CB-CG	5.73	118.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	192	THR	N-CA-C	5.72	117.84	108.52
1	M	137	ASN	CA-C-N	5.71	131.46	122.78
1	M	137	ASN	C-N-CA	5.71	131.46	122.78
1	M	192	TYR	N-CA-C	-5.70	99.13	108.41
2	J	44	ARG	CA-CB-CG	5.69	125.47	114.10
2	J	148	PHE	O-C-N	-5.68	116.26	122.06
1	L	161	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	M	185	GLU	CA-CB-CG	5.67	125.44	114.10
2	H	212	HIS	CA-C-N	5.67	125.14	119.24
2	H	212	HIS	C-N-CA	5.67	125.14	119.24
1	M	9	LEU	N-CA-C	-5.66	106.92	113.88
2	J	156	THR	N-CA-C	-5.66	100.81	109.41
2	J	148	PHE	CA-CB-CG	-5.65	108.15	113.80
2	H	153	THR	CA-CB-OG1	-5.64	101.13	109.60
1	L	163	TRP	CD2-CE2-CZ2	-5.63	116.77	122.40
1	L	114	THR	N-CA-C	-5.62	98.05	107.99
2	H	1	GLU	CB-CG-CD	5.61	122.14	112.60
1	M	171	SER	N-CA-CB	-5.61	103.72	112.41
1	M	90	GLN	CG-CD-NE2	5.60	124.81	116.40
2	J	87	THR	CA-CB-OG1	-5.59	101.21	109.60
1	L	50	LYS	CA-CB-CG	-5.59	102.92	114.10
1	M	35	TRP	O-C-N	5.57	129.83	123.31
1	L	25	SER	CA-C-O	-5.55	114.63	120.80
2	H	172	HIS	N-CA-C	-5.54	98.51	108.48
1	L	107	LYS	O-C-N	5.54	129.64	123.05
2	H	94	ARG	CB-CG-CD	-5.53	98.58	111.30
2	J	187	LEU	CA-CB-CG	5.52	135.62	116.30
1	L	207	LYS	CG-CD-CE	-5.51	98.62	111.30
2	J	36	TRP	CB-CG-CD1	-5.49	118.67	126.90
2	J	94	ARG	CA-CB-CG	-5.49	103.12	114.10
1	L	61	ARG	N-CA-C	-5.47	99.14	110.80
2	H	57	THR	N-CA-CB	-5.47	101.34	111.13
1	L	196	ALA	O-C-N	-5.46	117.10	123.27
2	H	118	PRO	CA-C-N	5.46	125.45	120.21
2	H	118	PRO	C-N-CA	5.46	125.45	120.21
2	J	200	PRO	N-CD-CG	-5.45	95.02	103.20
2	H	150	GLU	CA-C-O	-5.45	114.76	120.70
1	M	27(A)	THR	CA-C-N	-5.45	105.21	117.20
1	M	171	SER	N-CA-C	5.45	119.51	112.86
2	H	168	SER	CA-CB-OG	5.45	122.00	111.10
2	H	3	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	J	81	GLN	N-CA-C	-5.44	99.86	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	175	MET	CG-SD-CE	-5.43	88.95	100.90
2	H	82(B)	SER	CA-CB-OG	5.43	121.96	111.10
1	L	174	SER	CA-CB-OG	-5.43	100.24	111.10
1	L	165	ASP	CA-CB-CG	5.42	118.02	112.60
2	H	100(C)	PHE	CA-CB-CG	5.40	119.20	113.80
2	H	127	GLY	N-CA-C	-5.35	100.51	113.18
2	H	83	ARG	O-C-N	-5.34	116.76	122.85
1	M	156	GLN	CA-C-N	5.33	130.17	122.44
1	M	156	GLN	C-N-CA	5.33	130.17	122.44
2	H	217	THR	N-CA-C	-5.33	101.78	110.20
1	M	138	ASN	CA-CB-CG	5.33	117.93	112.60
2	H	81	GLN	CG-CD-NE2	5.33	124.39	116.40
2	H	122	TYR	CA-C-N	5.33	125.49	119.90
2	H	122	TYR	C-N-CA	5.33	125.49	119.90
1	M	124	GLN	OE1-CD-NE2	-5.33	117.28	122.60
1	M	154	GLU	N-CA-C	-5.32	99.10	108.20
2	J	123	PRO	CB-CA-C	5.32	117.33	111.11
2	H	57	THR	CA-CB-CG2	5.31	119.53	110.50
1	M	124	GLN	CG-CD-NE2	5.31	124.36	116.40
2	H	40	THR	CA-C-N	5.30	126.47	119.84
2	H	40	THR	C-N-CA	5.30	126.47	119.84
2	H	42	GLU	CB-CG-CD	5.29	121.60	112.60
1	L	51	VAL	N-CA-C	5.29	120.35	109.34
2	J	206	THR	CA-CB-OG1	-5.29	101.67	109.60
1	L	194	CYS	N-CA-CB	-5.28	102.31	110.65
2	H	173	THR	N-CA-C	-5.27	99.83	108.41
2	H	193	VAL	CA-C-N	5.24	125.24	119.89
2	H	193	VAL	C-N-CA	5.24	125.24	119.89
2	J	209	ASN	CA-CB-CG	5.24	117.84	112.60
1	M	76	SER	CA-CB-OG	-5.24	100.62	111.10
2	J	85	GLU	CA-CB-CG	5.24	124.58	114.10
1	L	153	SER	O-C-N	5.23	128.34	122.32
1	L	20	SER	O-C-N	5.23	129.66	123.33
2	H	199	ARG	NE-CZ-NH1	5.22	126.72	121.50
2	J	30	SER	N-CA-CB	-5.21	102.73	110.60
1	L	104	LEU	CA-CB-CG	5.21	134.52	116.30
1	L	48	ILE	N-CA-CB	-5.20	103.93	111.52
1	L	75	ILE	N-CA-C	-5.19	100.41	107.99
1	M	129	GLY	N-CA-C	-5.19	103.23	110.96
2	H	192	THR	CA-C-O	5.18	126.02	120.32
2	H	86	ASP	CA-CB-CG	-5.17	107.43	112.60
2	J	175	PRO	N-CA-C	5.17	119.69	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	119	PRO	N-CA-C	5.17	117.01	110.70
1	M	70	ASP	CA-CB-CG	5.17	117.77	112.60
2	J	133	GLN	CG-CD-NE2	5.17	124.15	116.40
2	J	48	VAL	N-CA-C	5.17	120.08	109.34
2	H	198	PRO	CA-N-CD	-5.16	104.77	112.00
1	M	145	ASN	CA-CB-CG	-5.13	107.47	112.60
1	M	126	THR	CA-CB-OG1	-5.13	101.90	109.60
2	H	110	THR	N-CA-C	-5.13	100.09	108.76
1	L	189	HIS	N-CA-CB	-5.12	102.82	110.60
2	H	166	LEU	N-CA-C	-5.11	98.92	108.02
2	J	45	LEU	N-CA-C	5.11	118.14	109.76
1	M	2	VAL	CA-C-N	-5.11	115.90	123.05
1	M	2	VAL	C-N-CA	-5.11	115.90	123.05
1	L	158	GLY	O-C-N	-5.11	116.06	122.70
1	L	69	THR	CA-CB-CG2	5.11	119.18	110.50
2	H	51	ILE	O-C-N	5.09	128.69	123.05
1	L	143	ASP	CA-CB-CG	-5.08	107.52	112.60
1	L	143	ASP	N-CA-C	5.08	117.52	109.96
2	J	32	CYS	N-CA-CB	-5.08	102.60	110.57
2	H	139	THR	O-C-N	5.07	129.55	123.36
1	M	104	LEU	N-CA-C	-5.07	101.50	109.25
2	H	13	LYS	CA-C-N	5.05	126.15	119.84
2	H	13	LYS	C-N-CA	5.05	126.15	119.84
2	J	94	ARG	N-CA-C	-5.05	101.17	109.40
1	L	189	HIS	CB-CG-ND1	5.05	130.27	122.70
1	L	55	PHE	N-CA-C	-5.05	104.20	110.41
2	J	162	ASN	CA-C-O	5.04	127.92	122.03
2	H	3	GLN	CG-CD-NE2	5.03	123.94	116.40
2	J	63	VAL	N-CA-C	-5.03	107.04	113.22
2	J	174	PHE	CA-CB-CG	-5.03	108.77	113.80
2	J	1	GLU	CB-CG-CD	5.02	121.14	112.60
2	J	19	LYS	CB-CG-CD	-5.01	99.78	111.30

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 ⓘ

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	52	0
1	M	1697	0	1639	43	0
2	H	1646	0	1614	34	0
2	J	1646	0	1614	43	0
3	L	14	0	13	0	0
All	All	6700	0	6518	165	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 (165) 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:HH11	2:H:199:ARG:HB3	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
1:M:4:MET:HE1	1:M:90:GLN:HB2	1.72	0.72
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:27(C):LEU:CB	1:M:68:GLY:HA2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:119:PRO:HB3	1:M:209:PHE:CE2	2.37	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:29:PHE:HE1	2:J:34:MET:HE2	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:NH1	2:J:199:ARG:O	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
1:M:49:TYR:CE1	1:M:53:ASN:HB2	2.42	0.54
2:J:199:ARG:HB3	2:J:200:PRO:HD3	1.89	0.54
2:H:194:PRO:O	2:H:198:PRO:HD2	2.06	0.54
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:H:20:LEU:HG	2:H:82:MET:HE2	1.88	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
1:L:132:VAL:HG13	1:L:179:LEU:HB3	1.88	0.53
2:H:12:VAL:O	2:H:111:VAL:HA	2.08	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:L:148:TRP:CE3	1:L:179:LEU:HD12	2.44	0.52
2:J:35:SER:HB2	2:J:95:TYR:CE2	2.45	0.52
2:H:199:ARG:HB3	2:H:199:ARG:NH1	2.10	0.52
1:M:27(C):LEU:HB2	1:M:68:GLY:HA2	1.92	0.52
1:M:4:MET:CE	1:M:90:GLN:HB2	2.39	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:J:174:PHE:O	2:J:187:LEU:HD22	2.12	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
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
2:J:1:GLU:O	2:J:26:GLY:HA3	2.12	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
2:H:82:MET:HE1	2:H:109:LEU:HD22	1.94	0.48
2:J:209:ASN:HB3	2:J:218:LYS:HZ3	1.78	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
1:M:2:VAL:O	1:M:97:THR:HG21	2.15	0.47
2:J:24:ALA:HB1	2:J:27:PHE:CE1	2.48	0.47
2:J:27:PHE:CE2	2:J:94:ARG:HD2	2.50	0.47
2:H:143:LEU:HD13	2:H:145:LYS:HB2	1.96	0.47
1:L:124:GLN:HE22	1:L:131:SER:H	1.62	0.46
2:H:140:LEU:HD11	2:H:199:ARG:HG3	1.97	0.46
1:M:150:ILE:HA	1:M:191:SER:O	2.16	0.46
2:J:33:ALA:O	2:J:95:TYR:HB2	2.15	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
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:121:VAL:HA	2:J:143:LEU:O	2.15	0.46
1:L:9:LEU:H	1:L:9:LEU:CD1	2.30	0.45
2:J:67:PHE:CD1	2:J:82:MET:HA	2.51	0.45
2:H:140:LEU:HD22	2:H:140:LEU:N	2.31	0.45
1:M:12:PRO:HA	1:M:105:GLU:O	2.17	0.45
2:J:176:ALA:HA	2:J:186:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:196:ALA:HB3	1:M:205:ILE:HB	1.98	0.45
1:M:66:GLY:HA3	1:M:71:PHE:HA	1.99	0.45
2:J:30:SER:HB3	2:J:73:ASN:HD22	1.82	0.45
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.51	0.45
1:L:34:GLU:HG3	1:L:49:TYR:HA	1.98	0.45
1:L:135:PHE:HB3	1:L:137:ASN:HD21	1.82	0.45
1:L:144:ILE:HG13	1:L:198:HIS:HB2	1.99	0.44
2:H:72:ASN:O	2:H:74:ALA:N	2.50	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: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:M:160:LEU:HG	2:J:177:VAL:HG11	1.99	0.44
1:M:207:LYS:HZ2	2:J:128:SER:HB3	1.83	0.44
1:L:35:TRP:HD1	1:L:48:ILE:CG2	2.31	0.43
2:J:80:LEU:HD23	2:J:80:LEU:HA	1.83	0.43
2:J:38:ARG:HH11	2:J:38:ARG:HD3	1.63	0.43
1:L:22:SER:HB2	1:L:24:ARG:HH12	1.84	0.43
2:J:29:PHE:CE1	2:J:34:MET:HE2	2.52	0.43
2:J:215:SER:O	2:J:217:THR:N	2.51	0.43
2:J:126:PRO:HG3	2:J:199:ARG:HD3	2.00	0.43
1:L:195:GLU:HG3	1:L:206:VAL:HG22	2.01	0.42
2:J:163:SER:N	2:J:209:ASN:HD21	2.12	0.42
1:M:54:ARG:HD3	1:M:62:PHE:O	2.20	0.42
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
2:H:124:LEU:HB2	2:H:141:GLY:C	2.44	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
1:L:151:ASP:C	1:L:153:SER:H	2.28	0.41
2:H:83:ARG:H	2:H:83:ARG:HG2	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:2:VAL:HG13	1:L:27:GLN:HB3	2.03	0.41
1:L:17:ASP:O	1:L:78:VAL:HG23	2.19	0.41
1:L:44:PRO:HD2	2:H:103:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:94:ARG:HH21	2:J:101:ASP:CG	2.29	0.41
2:H:126:PRO:HD3	2:H:140:LEU:HD12	2.03	0.41
1:M:19:ALA:O	1:M:74:LYS:HA	2.21	0.41
1:M:95:PRO:HA	1:M:96:PRO:HD3	1.94	0.41
1:M:124:GLN:HE22	1:M:131:SER:HB2	1.86	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: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
1:L:11:LEU:HA	1:L:12:PRO:HD3	1.88	0.40
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.56	0.40
2:H:143:LEU:CD1	2:H:145:LYS:HD2	2.51	0.40
1:L:15:LEU:HD21	1:L:80:ALA:HA	2.03	0.40
1:L:108:ARG:HD3	1:L:109:ALA:O	2.20	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%)	5	18
1	M	217/219 (99%)	195 (90%)	15 (7%)	7 (3%)	3	11
2	H	216/221 (98%)	186 (86%)	20 (9%)	10 (5%)	2	6
2	J	216/221 (98%)	185 (86%)	22 (10%)	9 (4%)	2	7
All	All	866/880 (98%)	762 (88%)	73 (8%)	31 (4%)	2	10

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
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 ⓘ

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%)	163 (83%)	33 (17%)	2	8
1	M	196/196 (100%)	166 (85%)	30 (15%)	3	10
2	H	189/192 (98%)	147 (78%)	42 (22%)	1	3
2	J	189/192 (98%)	155 (82%)	34 (18%)	2	6
All	All	770/776 (99%)	631 (82%)	139 (18%)	2	6

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	VAL
1	L	3	LEU
1	L	5	THR
1	L	7	THR
1	L	9	LEU
1	L	18	GLN
1	L	20	SER
1	L	22	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
1	L	81	GLU
1	L	97	THR
1	L	104	LEU
1	L	108	ARG
1	L	116	SER
1	L	126	THR
1	L	132	VAL
1	L	133	VAL
1	L	159	VAL
1	L	160	LEU
1	L	172	THR
1	L	179	LEU
1	L	185	GLU
1	L	191	SER
1	L	197	THR
1	L	202	THR
1	L	214	CYS

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Mol	Chain	Res	Type
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	68	ILE
2	H	72	ASN
2	H	73	ASN
2	H	82	MET
2	H	82(A)	SER
2	H	82(B)	SER
2	H	82(C)	LEU
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
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	215	SER
2	H	216	SER
2	H	217	THR

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Mol	Chain	Res	Type
1	M	2	VAL
1	M	4	MET
1	M	9	LEU
1	M	13	VAL
1	M	18	GLN
1	M	20	SER
1	M	23	CYS
1	M	24	ARG
1	M	43	SER
1	M	63	SER
1	M	69	THR
1	M	85	VAL
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	160	LEU
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
1	M	211	ARG
1	M	212	ASN
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	42	GLU
2	J	56	TYR
2	J	68	ILE
2	J	75	ARG

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Mol	Chain	Res	Type
2	J	83	ARG
2	J	85	GLU
2	J	87	THR
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	166	LEU
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
2	J	218	LYS
2	J	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	124	GLN
1	L	137	ASN
1	L	138	ASN
1	L	145	ASN
1	L	161	ASN
1	L	212	ASN
2	H	3	GLN
2	H	172	HIS
1	M	124	GLN
1	M	138	ASN
2	J	76	ASN
2	J	135	ASN
2	J	179	GLN
2	J	209	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.66	3 (17%)

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	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	901	NAG	O5-C1-C2	-4.66	104.08	111.29
3	L	901	NAG	C1-O5-C5	3.87	117.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	901	NAG	C1-C2-N2	2.17	113.85	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	901	NAG	C3-C2-N2-C7
3	L	901	NAG	C1-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.