Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 04:32 PM EDT

PDB ID	:	1YUH
Title	:	FAB FRAGMENT
Authors	:	Yuhasz, S.C.; Amzel, L.M.; Parry, C.; Strand, M.
Deposited on	:	1996-01-30
Resolution	:	3.00 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:

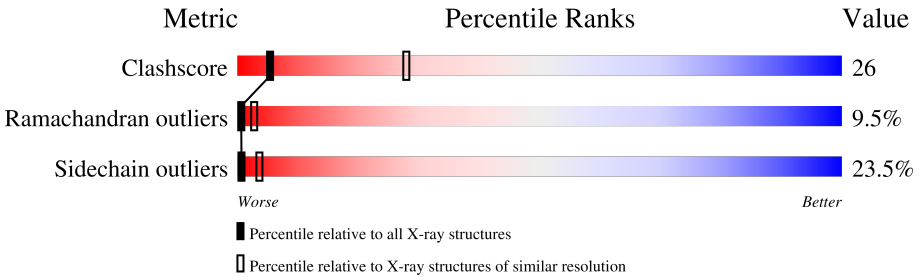
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	35% 41% 15% 9%
1	L	211	37% 39% 19% .
2	B	218	38% 40% 13% 9%
2	H	218	39% 44% 11% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6530 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 88C6/12 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1594	996	269	323	6			
1	A	211	Total	C	N	O	S	0	0	0
			1594	996	269	323	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	44	ARG	HIS	CONFLICT	GB 387376
L	57	GLY	ALA	CONFLICT	GB 387376
L	160	GLU	GLN	CONFLICT	GB 387376
L	184	SER	THR	CONFLICT	GB 387376
L	192	ALA	SER	CONFLICT	GB 387376
A	44	ARG	HIS	CONFLICT	GB 387376
A	57	GLY	ALA	CONFLICT	GB 387376
A	160	GLU	GLN	CONFLICT	GB 387376
A	184	SER	THR	CONFLICT	GB 387376
A	192	ALA	SER	CONFLICT	GB 387376

- Molecule 2 is a protein called 88C6/12 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1647	1046	273	319	9			
2	B	218	Total	C	N	O	S	0	0	0
			1647	1046	273	319	9			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	9	ALA	PRO	CONFLICT	GB 3399661
H	20	LEU	MET	CONFLICT	GB 3399661

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Chain	Residue	Modelled	Actual	Comment	Reference
H	33	LEU	VAL	CONFLICT	GB 3399661
H	37	ILE	VAL	CONFLICT	GB 3399661
H	40	ARG	LYS	CONFLICT	GB 3399661
H	43	ARG	GLN	CONFLICT	GB 3399661
H	50	ARG	TYR	CONFLICT	GB 3399661
H	52	ASP	ASN	CONFLICT	GB 3399661
H	54	ASN	TYR	CONFLICT	GB 3399661
H	56	VAL	ASP	CONFLICT	GB 3399661
H	57	VAL	GLY	CONFLICT	GB 3399661
H	60	PHE	TYR	CONFLICT	GB 3399661
H	66	SER	GLY	CONFLICT	GB 3399661
H	72	VAL	SER	CONFLICT	GB 3399661
H	75	PRO	SER	CONFLICT	GB 3399661
H	97	ALA	VAL	CONFLICT	GB 3399661
H	99	TYR	GLY	CONFLICT	GB 3399661
H	100	ALA	GLY	CONFLICT	GB 3399661
H	102	CYS	-	INSERTION	GB 3399661
H	?	-	TYR	DELETION	GB 3399661
H	?	-	TYR	DELETION	GB 3399661
H	?	-	ALA	DELETION	GB 3399661
H	113	THR	SER	CONFLICT	GB 3399661
H	120	ALA	LYS	CONFLICT	GB 3399661
H	163	ALA	SER	CONFLICT	GB 3399661
H	190	ALA	SER	CONFLICT	GB 3399661
H	196	GLY	GLU	CONFLICT	GB 3399661
H	210	ALA	LYS	CONFLICT	GB 3399661
B	9	ALA	PRO	CONFLICT	GB 3399661
B	20	LEU	MET	CONFLICT	GB 3399661
B	33	LEU	VAL	CONFLICT	GB 3399661
B	37	ILE	VAL	CONFLICT	GB 3399661
B	40	ARG	LYS	CONFLICT	GB 3399661
B	43	ARG	GLN	CONFLICT	GB 3399661
B	50	ARG	TYR	CONFLICT	GB 3399661
B	52	ASP	ASN	CONFLICT	GB 3399661
B	54	ASN	TYR	CONFLICT	GB 3399661
B	56	VAL	ASP	CONFLICT	GB 3399661
B	57	VAL	GLY	CONFLICT	GB 3399661
B	60	PHE	TYR	CONFLICT	GB 3399661
B	66	SER	GLY	CONFLICT	GB 3399661
B	72	VAL	SER	CONFLICT	GB 3399661
B	75	PRO	SER	CONFLICT	GB 3399661
B	97	ALA	VAL	CONFLICT	GB 3399661

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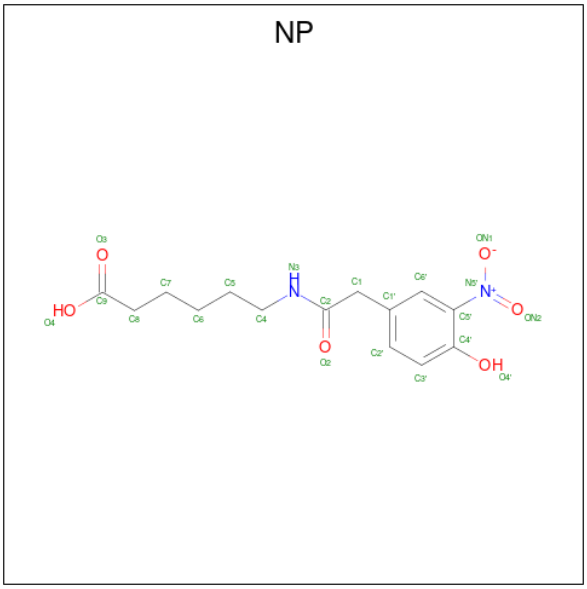
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	TYR	GLY	CONFLICT	GB 3399661
B	100	ALA	GLY	CONFLICT	GB 3399661
B	102	CYS	-	INSERTION	GB 3399661
B	?	-	TYR	DELETION	GB 3399661
B	?	-	TYR	DELETION	GB 3399661
B	?	-	ALA	DELETION	GB 3399661
B	113	THR	SER	CONFLICT	GB 3399661
B	120	ALA	LYS	CONFLICT	GB 3399661
B	163	ALA	SER	CONFLICT	GB 3399661
B	190	ALA	SER	CONFLICT	GB 3399661
B	196	GLY	GLU	CONFLICT	GB 3399661
B	210	ALA	LYS	CONFLICT	GB 3399661

- Molecule 3 is 4-HYDROXY-3-NITROPHENYLACETYL-EPSILON-AMINOCAPROIC ACID (three-letter code: NP) (formula: $C_{14}H_{18}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C N O 22 14 2 6	0	0
3	B	1	Total C N O 22 14 2 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O 1 1	0	0

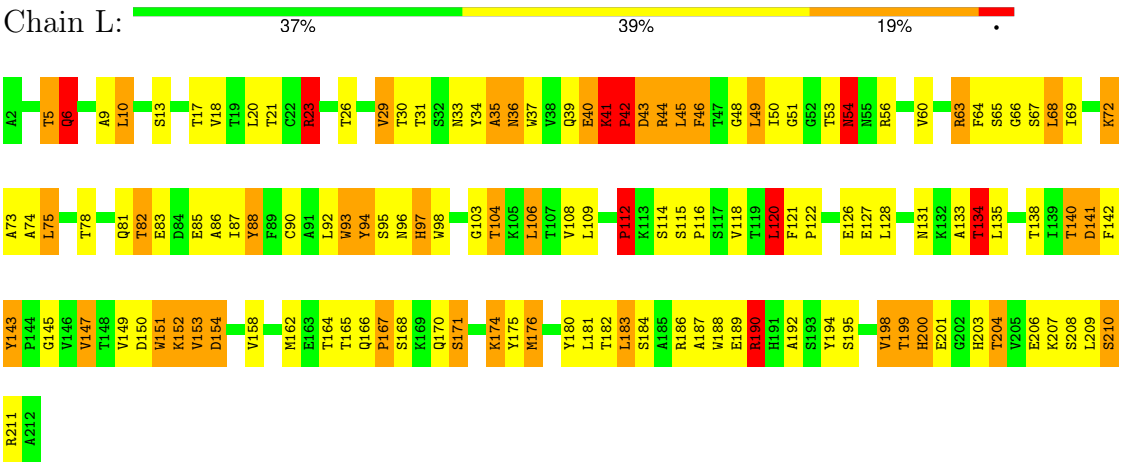
3 Residue-property plots (i)

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. 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.

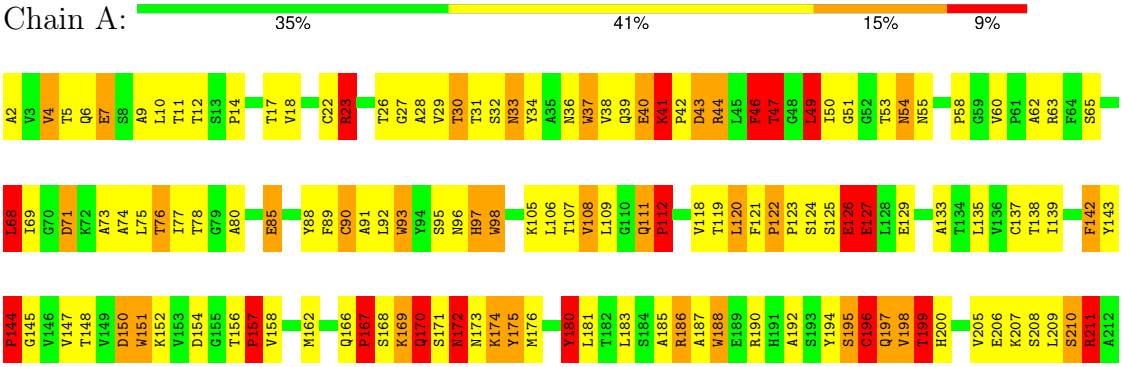
• Molecule 1: 88C6/12 FAB (LIGHT CHAIN)

Chain L:



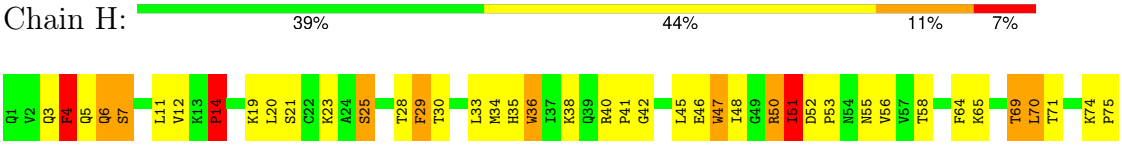
• Molecule 1: 88C6/12 FAB (LIGHT CHAIN)

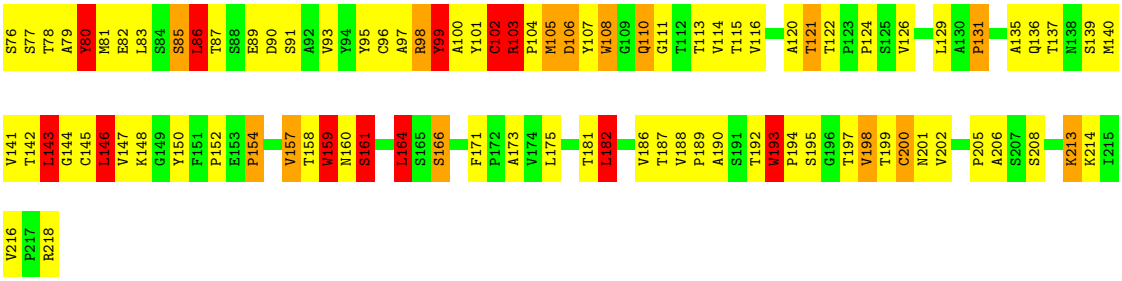
Chain A:



• Molecule 2: 88C6/12 FAB (HEAVY CHAIN)

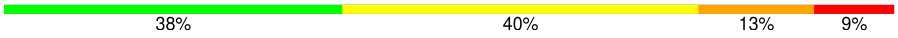
Chain H:

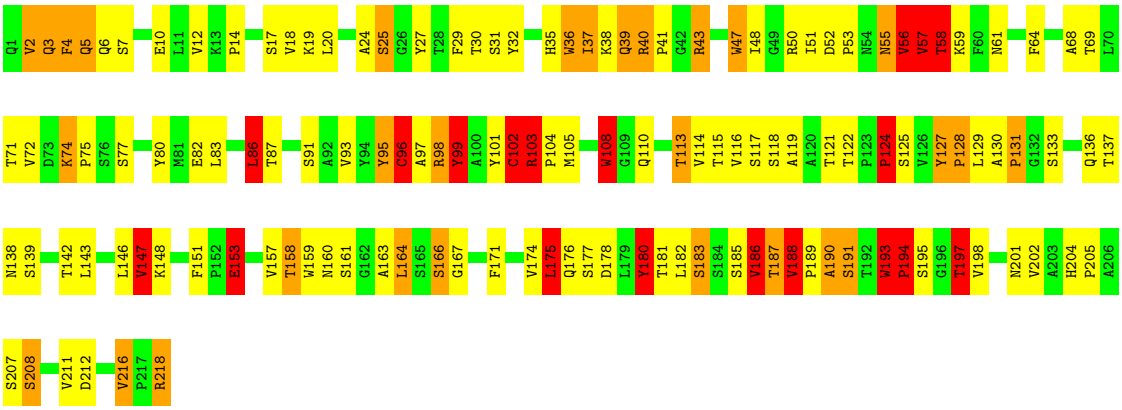




• Molecule 2: 88C6/12 FAB (HEAVY CHAIN)

Chain B:





4 Data and refinement statistics (i)

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	81.20Å 86.90Å 131.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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: NP

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	0.93	0/1630	2.06	55/2224 (2.5%)
1	L	0.93	0/1630	2.03	59/2224 (2.7%)
2	B	0.92	0/1691	2.10	64/2311 (2.8%)
2	H	0.92	0/1691	2.06	54/2311 (2.3%)
All	All	0.92	0/6642	2.06	232/9070 (2.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	6
2	H	0	2
All	All	0	14

There are no bond length outliers.

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	80	TYR	CB-CG-CD2	-12.10	113.74	121.00
1	L	190	ARG	NE-CZ-NH1	10.63	125.61	120.30
2	B	98	ARG	NE-CZ-NH2	-10.58	115.01	120.30
2	H	99	TYR	CB-CG-CD1	-10.56	114.66	121.00
2	B	36	TRP	CD1-CG-CD2	10.53	114.72	106.30
2	H	80	TYR	CB-CG-CD1	10.51	127.30	121.00
1	A	175	TYR	CB-CG-CD2	-10.44	114.74	121.00
2	H	108	TRP	CG-CD2-CE3	9.42	142.38	133.90
2	B	127	TYR	CB-CG-CD2	-9.26	115.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	159	TRP	CD1-CG-CD2	9.22	113.67	106.30
2	B	218	ARG	NE-CZ-NH2	-9.12	115.74	120.30
2	B	180	TYR	CB-CG-CD2	-9.01	115.59	121.00
2	H	146	LEU	CA-CB-CG	8.70	135.32	115.30
2	B	36	TRP	CE2-CD2-CG	-8.63	100.39	107.30
2	H	193	TRP	CD1-CG-CD2	8.60	113.18	106.30
2	B	98	ARG	NE-CZ-NH1	8.51	124.55	120.30
2	H	159	TRP	CE2-CD2-CG	-8.36	100.61	107.30
1	L	188	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	L	190	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	B	147	VAL	CA-CB-CG1	-8.20	98.60	110.90
1	L	37	TRP	CD1-CG-CD2	8.18	112.84	106.30
2	B	40	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	98	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	98	TRP	CE2-CD2-CG	-8.08	100.84	107.30
1	L	188	TRP	CE2-CD2-CG	-8.01	100.89	107.30
1	L	98	TRP	CD1-CG-CD2	7.96	112.67	106.30
2	H	193	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	L	189	GLU	N-CA-C	7.93	132.41	111.00
1	A	98	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	L	98	TRP	CE2-CD2-CG	-7.90	100.98	107.30
2	B	108	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	L	93	TRP	CD1-CG-CD2	7.83	112.57	106.30
2	B	164	LEU	N-CA-C	7.82	132.10	111.00
1	L	49	LEU	CA-CB-CG	7.79	133.22	115.30
2	H	80	TYR	CA-CB-CG	7.76	128.15	113.40
2	B	193	TRP	CE2-CD2-CG	-7.73	101.12	107.30
1	L	40	GLU	CA-CB-CG	7.69	130.32	113.40
1	L	151	TRP	CE2-CD2-CG	-7.67	101.16	107.30
2	H	98	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	L	45	LEU	CA-CB-CG	7.63	132.84	115.30
2	H	175	LEU	CA-CB-CG	7.60	132.78	115.30
2	H	47	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	A	188	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	93	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	L	37	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	98	TRP	CB-CG-CD1	-7.52	117.22	127.00
2	B	127	TYR	CB-CG-CD1	7.47	125.48	121.00
1	A	199	THR	CA-CB-CG2	7.43	122.80	112.40
2	H	198	VAL	CA-CB-CG2	-7.39	99.82	110.90
1	A	151	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	A	93	TRP	CE2-CD2-CG	-7.36	101.41	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	TYR	CB-CG-CD2	-7.34	116.59	121.00
2	B	108	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	H	108	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	H	47	TRP	CD1-CG-CD2	7.28	112.12	106.30
2	B	57	VAL	CG1-CB-CG2	-7.25	99.29	110.90
2	H	159	TRP	CG-CD2-CE3	7.22	140.40	133.90
1	A	5	THR	CA-C-N	-7.21	101.34	117.20
1	L	93	TRP	CE2-CD2-CG	-7.18	101.55	107.30
2	B	47	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	L	5	THR	CA-C-N	-7.12	101.54	117.20
2	H	85	SER	CA-C-N	-7.11	101.56	117.20
1	A	37	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	A	188	TRP	CG-CD2-CE3	7.08	140.27	133.90
2	B	153	GLU	N-CA-C	7.04	130.00	111.00
1	A	151	TRP	CD1-CG-CD2	6.98	111.88	106.30
1	A	175	TYR	CB-CG-CD1	6.96	125.18	121.00
2	B	175	LEU	CA-CB-CG	6.96	131.31	115.30
2	B	157	VAL	N-CA-CB	-6.92	96.28	111.50
2	B	157	VAL	N-CA-C	6.92	129.68	111.00
1	A	188	TRP	CB-CG-CD1	-6.89	118.04	127.00
1	A	151	TRP	CG-CD2-CE3	6.87	140.08	133.90
1	A	112	PRO	N-CA-C	6.83	129.87	112.10
2	B	193	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	L	88	TYR	CB-CG-CD1	-6.79	116.93	121.00
2	B	193	TRP	CG-CD2-CE3	6.77	140.00	133.90
2	B	159	TRP	CE2-CD2-CG	-6.72	101.92	107.30
2	B	208	SER	N-CA-C	6.72	129.14	111.00
2	H	36	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	180	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	A	37	TRP	CE2-CD2-CG	-6.68	101.96	107.30
2	H	51	ILE	CB-CA-C	-6.67	98.25	111.60
2	H	36	TRP	CD1-CG-CD2	6.63	111.60	106.30
2	B	96	CYS	CA-CB-SG	6.62	125.92	114.00
2	B	47	TRP	CD1-CG-CD2	6.58	111.57	106.30
1	A	170	GLN	CA-CB-CG	6.58	127.88	113.40
1	L	188	TRP	CG-CD2-CE3	6.48	139.73	133.90
1	A	23	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	H	108	TRP	CB-CG-CD1	-6.46	118.60	127.00
1	L	195	SER	N-CA-C	6.43	128.36	111.00
2	B	218	ARG	N-CA-C	6.42	128.32	111.00
1	L	151	TRP	CB-CG-CD1	-6.39	118.70	127.00
2	H	103	ARG	NE-CZ-NH2	-6.38	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	110	GLN	CA-CB-CG	6.37	127.41	113.40
1	L	176	MET	CG-SD-CE	-6.35	90.04	100.20
2	B	36	TRP	CG-CD1-NE1	-6.35	103.75	110.10
2	B	193	TRP	CB-CG-CD1	-6.33	118.77	127.00
1	A	4	VAL	CA-C-N	-6.30	103.34	117.20
1	L	198	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	A	211	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	159	TRP	CD1-CG-CD2	6.23	111.28	106.30
2	B	102	CYS	N-CA-C	6.23	127.82	111.00
2	H	166	SER	N-CA-C	6.21	127.76	111.00
1	L	56	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	63	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	L	98	TRP	CG-CD2-CE3	6.14	139.43	133.90
2	B	108	TRP	CG-CD2-CE3	6.13	139.41	133.90
1	L	151	TRP	CG-CD2-CE3	6.12	139.41	133.90
2	B	108	TRP	CA-CB-CG	6.10	125.30	113.70
1	A	188	TRP	CD1-CG-CD2	6.09	111.18	106.30
1	A	151	TRP	CB-CG-CD1	-6.06	119.12	127.00
2	H	65	LYS	O-C-N	-6.04	113.03	122.70
1	A	93	TRP	CG-CD2-CE3	6.02	139.31	133.90
1	L	118	VAL	CG1-CB-CG2	-6.01	101.29	110.90
1	L	23	ARG	CA-CB-CG	5.92	126.43	113.40
2	B	101	TYR	CA-CB-CG	5.92	124.65	113.40
1	A	167	PRO	N-CA-C	5.91	127.47	112.10
2	B	99	TYR	CA-CB-CG	5.91	124.63	113.40
2	H	202	VAL	CA-C-N	-5.88	104.26	117.20
2	H	4	PHE	CB-CG-CD2	-5.88	116.69	120.80
2	H	157	VAL	N-CA-C	5.86	126.83	111.00
1	A	172	ASN	CB-CG-ND2	5.86	130.76	116.70
1	A	46	PHE	N-CA-C	5.84	126.78	111.00
1	A	40	GLU	CA-CB-CG	5.83	126.22	113.40
2	H	159	TRP	CB-CG-CD1	-5.81	119.44	127.00
1	A	42	PRO	CA-N-CD	-5.80	103.38	111.50
2	B	36	TRP	CG-CD2-CE3	5.80	139.12	133.90
2	H	108	TRP	CA-CB-CG	5.80	124.72	113.70
2	B	122	THR	CA-CB-CG2	5.79	120.50	112.40
1	L	50	ILE	CA-CB-CG2	-5.78	99.34	110.90
1	L	151	TRP	CA-CB-CG	5.78	124.67	113.70
2	B	197	THR	N-CA-C	5.77	126.58	111.00
1	A	10	LEU	CA-CB-CG	5.77	128.57	115.30
2	B	95	TYR	N-CA-C	5.77	126.57	111.00
2	H	50	ARG	CA-CB-CG	5.76	126.08	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	88	TYR	CB-CG-CD1	-5.73	117.56	121.00
2	H	108	TRP	CD1-CG-CD2	5.73	110.88	106.30
1	L	211	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	86	LEU	N-CA-C	5.71	126.43	111.00
1	L	46	PHE	O-C-N	-5.69	113.59	122.70
1	L	153	VAL	CA-CB-CG2	-5.69	102.37	110.90
2	H	121	THR	CA-CB-CG2	5.68	120.35	112.40
1	A	49	LEU	CA-CB-CG	5.68	128.36	115.30
2	B	218	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	H	36	TRP	CG-CD2-CE3	5.66	138.99	133.90
1	A	126	GLU	CA-CB-CG	5.65	125.83	113.40
1	L	153	VAL	CA-CB-CG1	5.64	119.36	110.90
1	L	50	ILE	CA-CB-CG1	5.63	121.69	111.00
2	B	187	THR	N-CA-C	5.63	126.20	111.00
2	B	36	TRP	CB-CG-CD1	-5.60	119.72	127.00
2	H	198	VAL	CA-CB-CG1	5.59	119.29	110.90
1	L	188	TRP	CB-CG-CD1	-5.56	119.77	127.00
2	B	47	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	L	141	ASP	CB-CG-OD1	5.55	123.30	118.30
2	H	107	TYR	CB-CG-CD2	-5.54	117.68	121.00
2	H	7	SER	CA-C-N	5.53	127.27	116.20
1	A	43	ASP	N-CA-C	5.51	125.89	111.00
2	H	120	ALA	N-CA-C	5.51	125.88	111.00
2	B	43	ARG	N-CA-C	5.50	125.84	111.00
1	L	152	LYS	CA-CB-CG	5.49	125.49	113.40
1	L	43	ASP	CA-CB-CG	5.48	125.45	113.40
2	H	85	SER	N-CA-C	5.48	125.79	111.00
1	L	116	PRO	O-C-N	-5.47	113.95	122.70
1	L	114	SER	O-C-N	-5.47	113.95	122.70
2	H	154	PRO	N-CA-C	5.47	126.32	112.10
1	A	41	LYS	N-CA-C	5.47	125.76	111.00
1	A	172	ASN	OD1-CG-ND2	-5.46	109.33	121.90
1	L	171	SER	N-CA-C	5.46	125.75	111.00
1	A	62	ALA	CA-C-N	-5.46	105.19	117.20
1	L	134	THR	CA-C-N	-5.44	105.22	117.20
1	A	198	VAL	N-CA-CB	-5.44	99.54	111.50
2	H	197	THR	N-CA-C	5.42	125.63	111.00
2	B	58	THR	N-CA-C	5.42	125.63	111.00
1	L	10	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	102	CYS	CA-C-N	-5.42	105.28	117.20
1	L	42	PRO	CA-N-CD	-5.40	103.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	35	ALA	N-CA-C	5.37	125.51	111.00
2	B	124	PRO	N-CA-C	5.37	126.06	112.10
2	H	159	TRP	CG-CD1-NE1	-5.36	104.74	110.10
2	B	103	ARG	O-C-N	-5.34	110.95	121.10
1	L	195	SER	N-CA-CB	-5.33	102.51	110.50
2	B	194	PRO	N-CA-C	5.32	125.94	112.10
2	B	186	VAL	CA-CB-CG2	-5.32	102.93	110.90
1	L	94	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	B	191	SER	N-CA-C	5.30	125.30	111.00
1	A	195	SER	N-CA-C	5.29	125.30	111.00
2	B	188	VAL	N-CA-C	5.29	125.29	111.00
1	A	199	THR	CA-CB-OG1	-5.28	97.92	109.00
1	A	196	CYS	CA-CB-SG	5.27	123.48	114.00
2	B	163	ALA	N-CA-C	5.26	125.20	111.00
1	A	47	THR	N-CA-C	5.25	125.19	111.00
2	H	86	LEU	N-CA-C	5.25	125.17	111.00
2	H	182	LEU	CA-CB-CG	5.25	127.36	115.30
2	B	98	ARG	CA-CB-CG	5.24	124.93	113.40
2	H	28	THR	CA-C-N	-5.24	105.68	117.20
2	H	42	GLY	CA-C-N	5.22	128.68	117.20
1	L	116	PRO	N-CA-C	5.19	125.60	112.10
1	A	174	LYS	CA-C-N	5.19	128.61	117.20
2	B	51	ILE	CB-CA-C	-5.18	101.25	111.60
1	A	62	ALA	C-N-CA	5.17	134.64	121.70
1	A	197	GLN	CA-C-N	-5.16	105.84	117.20
2	B	190	ALA	C-N-CA	5.16	134.61	121.70
2	H	105	MET	CA-CB-CG	-5.16	104.53	113.30
2	H	86	LEU	CA-CB-CG	5.15	127.15	115.30
1	L	93	TRP	N-CA-CB	-5.15	101.33	110.60
2	H	198	VAL	N-CA-CB	-5.14	100.19	111.50
1	L	175	TYR	N-CA-C	5.14	124.88	111.00
2	B	122	THR	CA-CB-OG1	-5.12	98.25	109.00
1	A	170	GLN	N-CA-C	5.12	124.81	111.00
1	L	211	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	H	110	GLN	CG-CD-NE2	5.10	128.94	116.70
1	L	68	LEU	CA-CB-CG	5.09	127.00	115.30
1	L	5	THR	CA-C-O	5.08	130.77	120.10
1	A	151	TRP	CA-CB-CG	5.08	123.35	113.70
2	B	146	LEU	CA-CB-CG	5.08	126.97	115.30
2	H	143	LEU	CA-CB-CG	5.07	126.97	115.30
1	L	112	PRO	N-CA-C	5.07	125.27	112.10
1	L	120	LEU	CA-CB-CG	5.06	126.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	86	LEU	CA-CB-CG	5.05	126.93	115.30
1	L	127	GLU	CA-CB-CG	5.05	124.51	113.40
2	H	6	GLN	CA-CB-CG	-5.05	102.28	113.40
1	L	188	TRP	CG-CD1-NE1	-5.05	105.05	110.10
2	B	101	TYR	N-CA-C	-5.05	97.37	111.00
1	A	169	LYS	O-C-N	-5.04	114.63	122.70
1	L	49	LEU	CB-CG-CD2	-5.04	102.43	111.00
2	H	164	LEU	CA-CB-CG	5.04	126.89	115.30
2	B	147	VAL	CA-CB-CG2	5.04	118.45	110.90
1	L	54	ASN	N-CA-C	5.03	124.59	111.00
2	B	18	VAL	N-CA-C	5.03	124.58	111.00
1	A	196	CYS	CA-C-N	-5.02	106.16	117.20
1	A	44	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
1	A	143	TYR	Peptide
1	A	156	THR	Peptide
1	A	180	TYR	Sidechain
1	A	194	TYR	Sidechain
1	A	41	LYS	Peptide
2	B	103	ARG	Peptide
2	B	151	PHE	Peptide
2	B	171	PHE	Peptide
2	B	188	VAL	Peptide
2	B	193	TRP	Peptide
2	B	216	VAL	Peptide
2	H	193	TRP	Peptide
2	H	99	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1594	0	1538	96	0
1	L	1594	0	1538	80	0
2	B	1647	0	1622	98	0
2	H	1647	0	1622	107	0
3	B	22	0	16	2	0
3	H	22	0	16	1	0
4	H	1	0	0	0	0
4	L	3	0	0	0	0
All	All	6530	0	6352	337	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 26.

All (337) 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:A:150:ASP:HB2	1:A:197:GLN:HB3	1.38	1.02
2:H:105:MET:HG2	2:H:108:TRP:HE1	1.32	0.94
2:B:39:GLN:HB3	2:B:93:VAL:HB	1.55	0.88
2:H:19:LYS:HD2	2:H:80:TYR:HB3	1.57	0.86
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.58	0.86
1:A:37:TRP:HB2	1:A:50:ILE:HB	1.59	0.85
1:L:151:TRP:HD1	1:L:162:MET:SD	2.01	0.82
1:L:29:VAL:HG11	1:L:73:ALA:HB2	1.61	0.80
2:H:105:MET:HG2	2:H:108:TRP:NE1	1.96	0.80
2:H:30:THR:HA	2:H:53:PRO:HB2	1.66	0.78
2:H:5:GLN:HG2	2:H:23:LYS:HB3	1.64	0.77
2:H:69:THR:HG23	2:H:82:GLU:HB3	1.66	0.77
2:H:124:PRO:HB2	2:H:147:VAL:HG12	1.67	0.76
1:L:17:THR:HG22	1:L:78:THR:HA	1.66	0.76
1:A:49:LEU:HA	1:A:60:VAL:HG21	1.67	0.76
2:B:30:THR:HA	2:B:53:PRO:HB2	1.68	0.75
2:B:91:SER:OG	2:B:115:THR:HA	1.88	0.74
2:H:126:VAL:HB	2:H:147:VAL:HG13	1.70	0.74
1:L:151:TRP:CD1	1:L:162:MET:SD	2.82	0.73
1:L:20:LEU:HD13	1:L:75:LEU:HD23	1.69	0.73
1:L:85:GLU:HB2	1:L:108:VAL:HG22	1.71	0.73
1:L:82:THR:HA	1:L:108:VAL:HG21	1.70	0.72
2:H:38:LYS:HB3	2:H:48:ILE:HD11	1.70	0.71
2:H:99:TYR:HD1	2:H:103:ARG:HG3	1.54	0.71
2:B:202:VAL:HG12	2:B:211:VAL:O	1.90	0.71
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:HG22	2:B:82:GLU:HB3	1.72	0.70
1:L:48:GLY:HA3	2:H:105:MET:SD	2.31	0.69
1:A:120:LEU:HB3	1:A:137:CYS:HA	1.72	0.69
1:A:39:GLN:HB3	1:A:47:THR:HB	1.73	0.69
1:A:121:PHE:HB2	2:B:129:LEU:HD23	1.74	0.69
2:B:147:VAL:HG11	2:B:202:VAL:HG21	1.73	0.69
2:B:24:ALA:HB1	2:B:27:TYR:HE1	1.57	0.68
2:B:50:ARG:NH1	3:B:996:NP:H6'	2.07	0.68
1:L:190:ARG:HH11	1:L:190:ARG:HB3	1.59	0.68
1:A:133:ALA:HB3	1:A:183:LEU:HB2	1.77	0.67
1:A:135:LEU:HB2	1:A:181:LEU:HB3	1.77	0.67
2:B:74:LYS:HA	2:B:77:SER:HA	1.77	0.66
1:L:13:SER:HB3	1:L:109:LEU:HD23	1.77	0.65
1:L:97:HIS:HB2	2:H:47:TRP:CZ3	2.32	0.65
1:A:93:TRP:CZ2	1:A:96:ASN:HA	2.31	0.65
1:L:53:THR:HG21	1:L:68:LEU:HD12	1.77	0.65
1:L:54:ASN:HA	1:L:66:GLY:HA3	1.78	0.65
2:B:52:ASP:HB3	2:B:57:VAL:HB	1.80	0.64
2:B:3:GLN:NE2	2:B:5:GLN:HG3	2.13	0.64
2:H:173:ALA:HB2	2:H:182:LEU:HB2	1.79	0.64
1:A:2:ALA:N	1:A:26:THR:HG1	1.95	0.63
1:A:30:THR:HG23	1:A:32:SER:OG	1.98	0.63
2:B:27:TYR:CD2	2:B:32:TYR:HD2	2.16	0.63
1:L:33:ASN:O	1:L:93:TRP:HB3	1.98	0.63
1:A:152:LYS:HG2	1:A:157:PRO:HD3	1.80	0.63
1:A:118:VAL:HG22	1:A:139:ILE:HA	1.81	0.63
2:H:105:MET:SD	2:H:106:ASP:C	2.77	0.63
2:H:50:ARG:HH12	2:H:52:ASP:HB2	1.65	0.62
2:B:56:VAL:HG23	2:B:72:VAL:HG12	1.81	0.62
1:A:135:LEU:HD13	1:A:181:LEU:HG	1.81	0.62
2:H:105:MET:SD	2:H:105:MET:C	2.78	0.62
2:B:99:TYR:CE2	2:B:102:CYS:HA	2.34	0.62
1:A:185:ALA:HB3	1:A:186:ARG:HH12	1.65	0.62
1:L:85:GLU:HG3	1:L:106:LEU:O	2.00	0.61
1:L:97:HIS:HB2	2:H:47:TRP:HZ3	1.63	0.61
2:H:12:VAL:HG13	2:H:116:VAL:HG13	1.80	0.61
2:B:27:TYR:HD2	2:B:32:TYR:HD2	1.47	0.61
2:B:99:TYR:CZ	2:B:102:CYS:HA	2.35	0.61
1:A:145:GLY:HA3	1:A:175:TYR:CD2	2.36	0.61
1:A:151:TRP:O	1:A:157:PRO:HA	2.00	0.61
1:L:41:LYS:HG2	1:L:42:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HB3	2:H:51:ILE:HG13	1.81	0.61
2:H:74:LYS:HB2	2:H:75:PRO:HD3	1.83	0.61
2:H:157:VAL:HG23	2:H:201:ASN:O	2.01	0.61
1:A:127:GLU:HB3	2:B:127:TYR:CE2	2.36	0.61
2:H:5:GLN:OE1	2:H:25:SER:HB2	2.01	0.60
2:H:29:PHE:CE2	2:H:74:LYS:HA	2.36	0.60
1:L:122:PRO:HB2	2:H:218:ARG:HH12	1.65	0.60
2:H:19:LYS:HE3	2:H:82:GLU:HB2	1.83	0.60
2:B:97:ALA:HB1	2:B:105:MET:HB3	1.84	0.60
1:A:192:ALA:HB1	1:A:210:SER:OG	2.02	0.60
1:A:14:PRO:HA	1:A:80:ALA:O	2.02	0.60
1:A:36:ASN:HA	1:A:50:ILE:O	2.02	0.59
1:L:135:LEU:HB2	1:L:181:LEU:HB3	1.84	0.59
2:H:105:MET:SD	2:H:106:ASP:CA	2.90	0.59
1:A:12:THR:HG21	1:A:18:VAL:HB	1.84	0.59
2:B:55:ASN:ND2	2:B:57:VAL:HG23	2.17	0.59
1:A:198:VAL:HB	1:A:205:VAL:HB	1.84	0.59
1:L:199:THR:HG23	1:L:204:THR:HG23	1.84	0.59
2:H:50:ARG:NH1	2:H:52:ASP:HB2	2.16	0.59
1:A:107:THR:HG21	1:A:144:PRO:HG3	1.83	0.59
1:A:44:ARG:HH21	2:B:93:VAL:HG13	1.68	0.59
2:B:55:ASN:HD21	2:B:57:VAL:HG23	1.67	0.59
2:H:148:LYS:HG3	2:H:181:THR:HG23	1.85	0.59
1:A:183:LEU:HD22	1:A:187:ALA:HB1	1.85	0.59
2:H:99:TYR:HE1	2:H:102:CYS:N	2.01	0.59
1:L:121:PHE:CD2	2:H:129:LEU:HB3	2.37	0.59
2:H:52:ASP:HB3	2:H:55:ASN:OD1	2.03	0.59
2:B:143:LEU:HB2	2:B:186:VAL:HG12	1.85	0.58
1:A:120:LEU:HD11	1:A:208:SER:N	2.17	0.58
2:B:12:VAL:HG21	2:B:86:LEU:HD11	1.84	0.58
2:H:91:SER:OG	2:H:115:THR:HA	2.03	0.58
1:A:121:PHE:CD2	2:B:129:LEU:HB3	2.38	0.58
2:H:140:MET:HA	2:H:189:PRO:HA	1.84	0.58
2:H:105:MET:HG2	2:H:108:TRP:CD1	2.38	0.58
1:A:124:SER:HB3	2:B:129:LEU:HD12	1.83	0.58
2:H:33:LEU:HD11	2:H:50:ARG:HH11	1.69	0.58
1:A:53:THR:HG22	1:A:54:ASN:HD22	1.69	0.58
2:H:48:ILE:HA	2:H:64:PHE:HD2	1.68	0.57
2:H:105:MET:SD	2:H:106:ASP:N	2.78	0.57
1:A:38:VAL:HG23	1:A:89:PHE:HB2	1.87	0.57
1:A:29:VAL:HA	1:A:33:ASN:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:LEU:HB2	2:H:144:GLY:O	2.05	0.56
1:A:180:TYR:OH	2:B:183:SER:HB2	2.05	0.56
2:B:19:LYS:HD3	2:B:82:GLU:HB2	1.86	0.56
2:B:17:SER:HB3	2:B:83:LEU:O	2.06	0.56
2:H:105:MET:HE2	2:H:108:TRP:HD1	1.71	0.56
1:A:65:SER:HB2	1:A:76:THR:HB	1.86	0.56
2:H:3:GLN:HG2	2:H:25:SER:HB3	1.88	0.56
2:H:129:LEU:HA	2:H:218:ARG:NH2	2.21	0.56
2:H:161:SER:HA	2:H:201:ASN:OD1	2.06	0.56
2:B:40:ARG:HD3	2:B:41:PRO:HD3	1.88	0.56
1:L:147:VAL:HG23	1:L:200:HIS:HD2	1.70	0.55
1:L:164:THR:HG22	1:L:165:THR:N	2.21	0.55
2:H:48:ILE:HA	2:H:64:PHE:CD2	2.42	0.55
1:L:138:THR:HG23	2:H:171:PHE:HZ	1.70	0.55
1:A:34:TYR:CD1	2:B:102:CYS:HB2	2.41	0.55
1:L:49:LEU:HA	1:L:60:VAL:HG21	1.88	0.55
1:A:185:ALA:HB3	1:A:186:ARG:NH1	2.22	0.55
1:L:192:ALA:O	1:L:210:SER:HA	2.07	0.54
1:A:172:ASN:OD1	1:A:174:LYS:HE2	2.08	0.54
2:H:91:SER:HA	2:H:116:VAL:HG23	1.90	0.54
1:L:69:ILE:HG12	1:L:74:ALA:HB3	1.88	0.54
1:L:170:GLN:HG2	1:L:174:LYS:O	2.08	0.54
1:A:98:TRP:NE1	2:B:35:HIS:HE1	2.06	0.54
1:A:135:LEU:HD22	1:A:181:LEU:HD23	1.89	0.54
1:L:21:THR:HB	1:L:72:LYS:HD3	1.88	0.54
1:L:36:ASN:ND2	1:L:51:GLY:HA2	2.23	0.54
1:L:190:ARG:HB3	1:L:190:ARG:NH1	2.21	0.54
2:H:50:ARG:NE	3:H:995:NP:H11	2.23	0.53
1:A:126:GLU:O	1:A:129:GLU:HG2	2.07	0.53
2:H:12:VAL:HG21	2:H:86:LEU:HD21	1.89	0.53
2:B:167:GLY:HA3	2:B:187:THR:OG1	2.07	0.53
1:L:69:ILE:HB	1:L:72:LYS:HZ2	1.73	0.53
2:H:97:ALA:HA	2:H:108:TRP:HA	1.91	0.53
1:L:51:GLY:HA3	2:H:103:ARG:HH12	1.73	0.53
1:A:69:ILE:HG13	1:A:74:ALA:HB3	1.91	0.53
1:A:124:SER:OG	2:B:127:TYR:HB3	2.08	0.53
2:H:19:LYS:CE	2:H:82:GLU:HB2	2.38	0.53
1:A:50:ILE:HG13	1:A:75:LEU:HD12	1.90	0.53
1:L:51:GLY:HA3	2:H:103:ARG:NH1	2.24	0.53
1:L:40:GLU:O	1:L:86:ALA:HB1	2.09	0.53
1:L:190:ARG:HD2	1:L:190:ARG:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:TYR:CG	2:H:108:TRP:HE3	2.27	0.52
1:A:142:PHE:CD1	1:A:142:PHE:N	2.77	0.52
2:H:47:TRP:HZ2	2:H:50:ARG:HB2	1.75	0.52
1:A:46:PHE:HB3	2:B:108:TRP:NE1	2.24	0.52
1:L:9:ALA:HA	1:L:104:THR:HG22	1.90	0.52
1:L:63:ARG:HH12	1:L:81:GLN:HE21	1.58	0.52
1:A:190:ARG:HA	1:A:211:ARG:NH1	2.25	0.52
1:L:134:THR:HG21	2:H:148:LYS:NZ	2.24	0.52
1:A:118:VAL:HG21	1:A:198:VAL:HG11	1.91	0.52
2:B:50:ARG:HH12	3:B:996:NP:H6'	1.73	0.52
1:L:87:ILE:HA	1:L:104:THR:O	2.09	0.51
1:L:158:VAL:HG11	1:L:181:LEU:HD11	1.91	0.51
2:H:76:SER:O	2:H:78:THR:HG23	2.10	0.51
2:H:103:ARG:HG2	2:H:103:ARG:HH11	1.75	0.51
1:A:147:VAL:HG23	1:A:199:THR:O	2.11	0.51
1:L:85:GLU:HB2	1:L:108:VAL:CG2	2.41	0.51
1:A:142:PHE:N	1:A:142:PHE:HD1	2.08	0.51
2:B:50:ARG:O	2:B:58:THR:HA	2.10	0.51
2:B:193:TRP:CD1	2:B:194:PRO:HA	2.46	0.51
2:B:95:TYR:HB3	2:B:108:TRP:HE3	1.76	0.51
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.41	0.50
2:H:51:ILE:CD1	2:H:79:ALA:HB1	2.41	0.50
2:H:140:MET:HB3	2:H:187:THR:HG22	1.92	0.50
2:H:86:LEU:HD12	2:H:90:ASP:OD1	2.11	0.50
2:H:146:LEU:HD11	2:H:148:LYS:HD2	1.94	0.50
1:A:51:GLY:HA3	2:B:103:ARG:HH12	1.77	0.50
2:B:158:THR:O	2:B:201:ASN:HB2	2.12	0.50
2:B:50:ARG:HH21	2:B:59:LYS:HG3	1.77	0.50
2:H:36:TRP:HD1	2:H:70:LEU:HD21	1.76	0.49
2:B:117:SER:OG	2:B:119:ALA:HB3	2.12	0.49
1:A:36:ASN:OD1	2:B:103:ARG:HA	2.13	0.49
2:H:161:SER:HA	2:H:201:ASN:HD21	1.76	0.49
1:L:6:GLN:NE2	1:L:103:GLY:H	2.11	0.49
1:A:38:VAL:HG12	2:B:105:MET:SD	2.53	0.49
1:A:44:ARG:NH2	2:B:93:VAL:HG13	2.27	0.49
1:L:131:ASN:O	1:L:184:SER:HA	2.13	0.49
1:A:122:PRO:O	2:B:129:LEU:HG	2.12	0.49
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.77	0.49
2:B:153:GLU:HA	2:B:180:TYR:CE1	2.48	0.49
2:H:103:ARG:NH1	2:H:103:ARG:HG2	2.28	0.49
1:A:97:HIS:HA	2:B:47:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:TRP:CH2	2:H:200:CYS:SG	3.07	0.48
1:A:28:ALA:HB1	1:A:71:ASP:HB2	1.94	0.48
1:A:209:LEU:HD12	2:B:133:SER:OG	2.13	0.48
2:B:175:LEU:HB3	2:B:180:TYR:HD2	1.77	0.48
2:H:45:LEU:HD13	2:H:108:TRP:HH2	1.78	0.48
2:B:47:TRP:HZ2	2:B:50:ARG:HB2	1.77	0.48
2:B:193:TRP:HE1	2:B:198:VAL:H	1.60	0.48
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.32	0.48
2:H:99:TYR:CD1	2:H:103:ARG:HG3	2.42	0.48
1:A:120:LEU:HD21	1:A:207:LYS:O	2.14	0.48
1:A:111:GLN:HA	1:A:112:PRO:HD2	1.63	0.47
1:A:68:LEU:HA	1:A:73:ALA:HA	1.96	0.47
2:B:52:ASP:CB	2:B:57:VAL:HB	2.43	0.47
1:L:198:VAL:O	1:L:204:THR:HA	2.14	0.47
2:H:143:LEU:HD23	2:H:186:VAL:HG13	1.96	0.47
2:H:160:ASN:CB	2:H:164:LEU:HD22	2.44	0.47
1:L:147:VAL:HG23	1:L:200:HIS:CD2	2.48	0.47
2:H:14:PRO:HD3	2:H:116:VAL:HG12	1.96	0.47
1:A:29:VAL:HG22	1:A:92:LEU:HD21	1.97	0.47
1:A:147:VAL:HG22	1:A:148:THR:N	2.30	0.47
2:B:56:VAL:HG23	2:B:72:VAL:CG1	2.44	0.47
1:L:34:TYR:CB	2:H:102:CYS:SG	3.02	0.47
2:H:12:VAL:O	2:H:116:VAL:HA	2.15	0.47
2:B:87:THR:O	2:B:116:VAL:HG11	2.14	0.47
2:B:131:PRO:HD2	2:B:143:LEU:HD13	1.96	0.47
2:H:161:SER:HA	2:H:201:ASN:ND2	2.30	0.47
1:A:38:VAL:CG2	1:A:89:PHE:HB2	2.45	0.47
1:L:164:THR:HG22	1:L:165:THR:H	1.80	0.47
1:A:4:VAL:HG13	1:A:22:CYS:SG	2.55	0.47
2:B:147:VAL:HG11	2:B:202:VAL:CG2	2.44	0.47
1:L:46:PHE:O	2:H:105:MET:HE3	2.15	0.46
1:A:170:GLN:NE2	1:A:176:MET:HG2	2.30	0.46
1:L:44:ARG:HH12	2:H:111:GLY:HA3	1.80	0.46
2:B:142:THR:HA	2:B:186:VAL:O	2.15	0.46
2:B:5:GLN:HE22	2:B:25:SER:HB2	1.81	0.46
2:H:33:LEU:HD23	2:H:99:TYR:OH	2.16	0.46
2:H:12:VAL:HG12	2:H:114:VAL:HG22	1.98	0.46
1:A:29:VAL:HA	1:A:33:ASN:ND2	2.30	0.46
2:B:4:PHE:CE2	2:B:96:CYS:SG	3.09	0.46
1:A:53:THR:HG23	1:A:68:LEU:HB2	1.98	0.46
1:L:49:LEU:HD11	1:L:64:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:TRP:HD1	2:H:198:VAL:HB	1.80	0.46
1:L:88:TYR:O	1:L:103:GLY:HA2	2.16	0.45
1:A:120:LEU:HD23	1:A:196:CYS:HB3	1.97	0.45
2:H:33:LEU:HD11	2:H:50:ARG:NH1	2.32	0.45
2:B:124:PRO:HB2	2:B:147:VAL:CG1	2.46	0.45
1:L:72:LYS:HZ3	1:L:74:ALA:HB2	1.82	0.45
1:L:135:LEU:O	1:L:180:TYR:HA	2.17	0.45
2:H:160:ASN:H	2:H:164:LEU:CD2	2.30	0.45
2:H:160:ASN:H	2:H:164:LEU:HD22	1.81	0.45
1:A:40:GLU:HG2	1:A:89:PHE:HE2	1.81	0.45
2:B:125:SER:O	2:B:148:LYS:HB2	2.16	0.45
1:A:4:VAL:CG1	1:A:22:CYS:SG	3.04	0.45
2:H:38:LYS:HG2	2:H:46:GLU:HB2	1.98	0.45
2:B:95:TYR:HB3	2:B:108:TRP:CE3	2.51	0.45
2:H:126:VAL:O	2:H:213:LYS:HD3	2.17	0.45
2:B:188:VAL:HA	2:B:189:PRO:HD2	1.76	0.45
2:B:99:TYR:CD2	2:B:103:ARG:O	2.69	0.45
1:L:184:SER:O	1:L:187:ALA:HB3	2.17	0.44
1:A:11:THR:HG21	1:A:109:LEU:HD12	1.98	0.44
1:L:36:ASN:ND2	2:H:103:ARG:HA	2.32	0.44
1:L:142:PHE:HB2	1:L:200:HIS:NE2	2.33	0.44
2:H:87:THR:OG1	2:H:89:GLU:HB2	2.18	0.44
2:B:37:ILE:HG21	2:B:108:TRP:HZ3	1.82	0.44
1:L:166:GLN:HG2	1:L:167:PRO:HG2	2.00	0.44
2:H:19:LYS:HD2	2:H:80:TYR:CB	2.39	0.44
1:A:18:VAL:HG12	1:A:80:ALA:HB2	1.99	0.44
2:B:204:HIS:CE1	2:B:207:SER:OG	2.70	0.44
1:L:142:PHE:HB2	1:L:200:HIS:CE1	2.53	0.44
2:B:99:TYR:HD2	2:B:103:ARG:O	2.00	0.44
2:H:51:ILE:HD11	2:H:79:ALA:HB1	2.00	0.44
2:B:193:TRP:CD1	2:B:197:THR:HA	2.53	0.44
1:L:183:LEU:HD21	1:L:194:TYR:HE2	1.82	0.44
2:H:81:MET:HG2	2:H:83:LEU:CD1	2.47	0.43
2:B:124:PRO:HB2	2:B:147:VAL:HG12	2.00	0.43
1:A:142:PHE:HE2	1:A:147:VAL:HG11	1.82	0.43
1:A:36:ASN:CG	2:B:103:ARG:HA	2.39	0.43
2:B:29:PHE:CD2	2:B:74:LYS:HB3	2.53	0.43
2:B:30:THR:CG2	2:B:74:LYS:HG2	2.49	0.43
1:L:48:GLY:CA	2:H:105:MET:SD	3.02	0.43
1:L:153:VAL:HG22	1:L:194:TYR:CE2	2.54	0.43
2:B:130:ALA:HA	2:B:131:PRO:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:PHE:CE2	2:H:45:LEU:HD11	2.54	0.43
2:B:71:THR:O	2:B:80:TYR:HB2	2.18	0.43
2:B:131:PRO:CD	2:B:143:LEU:HD13	2.49	0.43
2:H:33:LEU:HD23	2:H:99:TYR:CZ	2.54	0.42
2:H:50:ARG:O	2:H:58:THR:HA	2.18	0.42
2:H:126:VAL:HA	2:H:146:LEU:O	2.18	0.42
1:A:44:ARG:NH2	2:B:113:THR:HG23	2.34	0.42
1:A:170:GLN:HG2	1:A:172:ASN:ND2	2.34	0.42
2:B:4:PHE:HE2	2:B:96:CYS:SG	2.43	0.42
2:H:141:VAL:HG12	2:H:188:VAL:O	2.19	0.42
2:B:61:ASN:HB3	2:B:64:PHE:HB2	2.00	0.42
1:L:166:GLN:HA	1:L:167:PRO:HD2	1.79	0.42
2:H:36:TRP:HA	2:H:95:TYR:O	2.20	0.42
1:A:127:GLU:HB3	2:B:127:TYR:CZ	2.54	0.42
2:B:36:TRP:CH2	2:B:96:CYS:HB3	2.55	0.42
1:A:172:ASN:OD1	1:A:174:LYS:HB2	2.19	0.42
1:L:121:PHE:O	1:L:209:LEU:HD11	2.20	0.42
2:H:6:GLN:HG3	2:H:21:SER:O	2.20	0.42
1:A:133:ALA:O	1:A:135:LEU:HD12	2.20	0.42
2:B:125:SER:N	2:B:148:LYS:O	2.53	0.42
2:B:148:LYS:HG2	2:B:181:THR:HG23	2.02	0.42
2:B:195:SER:O	2:B:197:THR:N	2.52	0.42
1:L:6:GLN:HE21	1:L:6:GLN:HB2	1.74	0.41
1:L:121:PHE:HD2	2:H:129:LEU:HB3	1.85	0.41
1:A:11:THR:HG22	1:A:12:THR:N	2.35	0.41
1:A:151:TRP:HA	1:A:195:SER:O	2.20	0.41
1:L:34:TYR:HB2	2:H:102:CYS:SG	2.61	0.41
1:L:5:THR:N	1:L:23:ARG:O	2.53	0.41
1:L:134:THR:HG21	2:H:148:LYS:HZ3	1.85	0.41
2:H:93:VAL:HA	2:H:113:THR:HA	2.02	0.41
1:A:85:GLU:OE2	1:A:108:VAL:HG23	2.20	0.41
2:H:4:PHE:HE1	2:H:96:CYS:SG	2.44	0.41
1:A:170:GLN:O	1:A:172:ASN:N	2.53	0.41
1:L:133:ALA:HB3	1:L:183:LEU:HD12	2.02	0.41
1:L:199:THR:HG22	1:L:203:HIS:N	2.35	0.41
1:A:22:CYS:HB3	1:A:73:ALA:HB3	2.03	0.41
1:A:98:TRP:CD1	2:B:35:HIS:HE1	2.38	0.41
1:A:158:VAL:HG11	1:A:181:LEU:HD13	2.02	0.41
2:B:136:GLN:O	2:B:138:ASN:N	2.53	0.41
1:L:143:TYR:HD2	1:L:174:LYS:HG3	1.85	0.41
1:A:34:TYR:HB3	2:B:102:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:NZ	1:A:197:GLN:NE2	2.69	0.41
2:B:3:GLN:HE21	2:B:5:GLN:HG3	1.85	0.41
2:H:199:THR:OG1	2:H:214:LYS:HG2	2.21	0.41
1:A:36:ASN:ND2	2:B:103:ARG:HA	2.36	0.41
1:A:44:ARG:HH21	2:B:93:VAL:CG1	2.33	0.41
1:L:120:LEU:HD13	1:L:151:TRP:CH2	2.56	0.41
1:L:122:PRO:HB2	2:H:218:ARG:NH1	2.34	0.41
1:A:9:ALA:HB1	1:A:105:LYS:HB2	2.03	0.41
2:B:193:TRP:CG	2:B:194:PRO:HA	2.56	0.41
1:L:140:THR:O	1:L:141:ASP:HB2	2.21	0.41
1:A:197:GLN:HB2	1:A:206:GLU:OE1	2.21	0.41
2:B:10:GLU:HB2	2:B:114:VAL:HG22	2.03	0.41
1:L:34:TYR:HB3	2:H:102:CYS:SG	2.61	0.40
1:L:96:ASN:O	1:L:97:HIS:HB3	2.21	0.40
1:A:18:VAL:HG13	1:A:77:ILE:HB	2.03	0.40
1:A:90:CYS:SG	1:A:91:ALA:N	2.94	0.40
2:B:2:VAL:HG11	2:B:98:ARG:HH12	1.85	0.40
2:B:68:ALA:HA	2:B:82:GLU:O	2.20	0.40
1:L:20:LEU:N	1:L:75:LEU:O	2.54	0.40
2:H:131:PRO:HG3	2:H:143:LEU:HD13	2.03	0.40
1:A:123:PRO:HG3	1:A:135:LEU:HG	2.04	0.40
2:B:127:TYR:HA	2:B:128:PRO:HD2	1.90	0.40
1:L:36:ASN:O	1:L:90:CYS:HA	2.22	0.40
2:H:193:TRP:CE3	2:H:194:PRO:HD3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	207/211 (98%)	149 (72%)	41 (20%)	17 (8%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	207/211 (98%)	164 (79%)	28 (14%)	15 (7%)	1 5
2	B	214/218 (98%)	155 (72%)	35 (16%)	24 (11%)	0 2
2	H	214/218 (98%)	167 (78%)	23 (11%)	24 (11%)	0 2
All	All	842/858 (98%)	635 (75%)	127 (15%)	80 (10%)	0 3

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	112	PRO
1	L	154	ASP
1	L	167	PRO
1	L	171	SER
2	H	7	SER
2	H	139	SER
1	A	41	LYS
1	A	47	THR
1	A	112	PRO
1	A	127	GLU
1	A	169	LYS
1	A	171	SER
1	A	210	SER
2	B	57	VAL
2	B	121	THR
2	B	137	THR
2	B	139	SER
2	B	160	ASN
2	B	166	SER
2	B	176	GLN
2	B	190	ALA
2	B	191	SER
2	B	205	PRO
1	L	95	SER
2	H	4	PHE
2	H	29	PHE
2	H	85	SER
2	H	100	ALA
2	H	102	CYS
2	H	135	ALA
2	H	137	THR
2	H	161	SER
1	A	43	ASP

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Mol	Chain	Res	Type
1	A	95	SER
1	A	167	PRO
2	B	7	SER
2	B	102	CYS
1	L	35	ALA
1	L	42	PRO
1	L	82	THR
1	L	145	GLY
2	H	41	PRO
2	H	56	VAL
2	H	121	THR
1	A	7	GLU
1	A	27	GLY
1	A	157	PRO
1	A	162	MET
2	B	194	PRO
1	L	6	GLN
1	L	29	VAL
1	L	41	LYS
2	H	131	PRO
2	H	154	PRO
2	H	190	ALA
2	H	195	SER
1	A	54	ASN
2	B	55	ASN
2	B	56	VAL
2	B	110	GLN
2	B	153	GLU
2	B	161	SER
2	B	177	SER
2	B	178	ASP
1	L	44	ARG
1	L	97	HIS
2	H	166	SER
2	H	205	PRO
2	H	206	ALA
2	B	208	SER
1	L	115	SER
2	H	77	SER
2	H	192	THR
2	H	208	SER
1	A	58	PRO

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Mol	Chain	Res	Type
1	A	144	PRO
2	B	128	PRO
2	H	14	PRO
2	B	131	PRO
2	B	124	PRO

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	177/177 (100%)	133 (75%)	44 (25%)	0 3
1	L	177/177 (100%)	127 (72%)	50 (28%)	0 2
2	B	185/185 (100%)	143 (77%)	42 (23%)	1 4
2	H	185/185 (100%)	151 (82%)	34 (18%)	1 9
All	All	724/724 (100%)	554 (76%)	170 (24%)	1 3

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	10	LEU
1	L	18	VAL
1	L	23	ARG
1	L	26	THR
1	L	30	THR
1	L	31	THR
1	L	36	ASN
1	L	39	GLN
1	L	41	LYS
1	L	43	ASP
1	L	45	LEU
1	L	54	ASN
1	L	63	ARG
1	L	65	SER
1	L	67	SER

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Mol	Chain	Res	Type
1	L	72	LYS
1	L	75	LEU
1	L	83	GLU
1	L	92	LEU
1	L	94	TYR
1	L	104	THR
1	L	106	LEU
1	L	112	PRO
1	L	120	LEU
1	L	126	GLU
1	L	128	LEU
1	L	134	THR
1	L	140	THR
1	L	143	TYR
1	L	147	VAL
1	L	149	VAL
1	L	150	ASP
1	L	152	LYS
1	L	154	ASP
1	L	168	SER
1	L	174	LYS
1	L	176	MET
1	L	182	THR
1	L	183	LEU
1	L	186	ARG
1	L	190	ARG
1	L	199	THR
1	L	200	HIS
1	L	201	GLU
1	L	204	THR
1	L	206	GLU
1	L	207	LYS
1	L	208	SER
1	L	210	SER
2	H	11	LEU
2	H	14	PRO
2	H	20	LEU
2	H	25	SER
2	H	40	ARG
2	H	51	ILE
2	H	69	THR
2	H	70	LEU

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Mol	Chain	Res	Type
2	H	71	THR
2	H	80	TYR
2	H	86	LEU
2	H	98	ARG
2	H	99	TYR
2	H	101	TYR
2	H	102	CYS
2	H	103	ARG
2	H	104	PRO
2	H	106	ASP
2	H	110	GLN
2	H	122	THR
2	H	136	GLN
2	H	142	THR
2	H	143	LEU
2	H	145	CYS
2	H	146	LEU
2	H	152	PRO
2	H	158	THR
2	H	159	TRP
2	H	161	SER
2	H	164	LEU
2	H	182	LEU
2	H	200	CYS
2	H	213	LYS
2	H	216	VAL
1	A	6	GLN
1	A	7	GLU
1	A	17	THR
1	A	23	ARG
1	A	30	THR
1	A	31	THR
1	A	33	ASN
1	A	46	PHE
1	A	49	LEU
1	A	55	ASN
1	A	68	LEU
1	A	71	ASP
1	A	76	THR
1	A	78	THR
1	A	85	GLU
1	A	90	CYS

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Mol	Chain	Res	Type
1	A	97	HIS
1	A	106	LEU
1	A	108	VAL
1	A	111	GLN
1	A	112	PRO
1	A	119	THR
1	A	120	LEU
1	A	125	SER
1	A	126	GLU
1	A	127	GLU
1	A	138	THR
1	A	142	PHE
1	A	144	PRO
1	A	150	ASP
1	A	154	ASP
1	A	157	PRO
1	A	166	GLN
1	A	167	PRO
1	A	168	SER
1	A	170	GLN
1	A	172	ASN
1	A	173	ASN
1	A	186	ARG
1	A	188	TRP
1	A	196	CYS
1	A	199	THR
1	A	200	HIS
1	A	211	ARG
2	B	2	VAL
2	B	3	GLN
2	B	4	PHE
2	B	5	GLN
2	B	6	GLN
2	B	14	PRO
2	B	20	LEU
2	B	25	SER
2	B	31	SER
2	B	37	ILE
2	B	39	GLN
2	B	43	ARG
2	B	56	VAL
2	B	58	THR

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Mol	Chain	Res	Type
2	B	74	LYS
2	B	75	PRO
2	B	86	LEU
2	B	96	CYS
2	B	99	TYR
2	B	104	PRO
2	B	108	TRP
2	B	113	THR
2	B	118	SER
2	B	147	VAL
2	B	153	GLU
2	B	158	THR
2	B	164	LEU
2	B	166	SER
2	B	174	VAL
2	B	175	LEU
2	B	180	TYR
2	B	182	LEU
2	B	183	SER
2	B	185	SER
2	B	186	VAL
2	B	188	VAL
2	B	193	TRP
2	B	194	PRO
2	B	197	THR
2	B	212	ASP
2	B	216	VAL
2	B	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	81	GLN
1	L	200	HIS
2	H	35	HIS
2	H	54	ASN
1	A	39	GLN
1	A	54	ASN
1	A	197	GLN
2	B	3	GLN
2	B	35	HIS
2	B	204	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NP	H	995	-	22,22,22	1.69	2 (9%)	24,28,28	9.01	8 (33%)
3	NP	B	996	-	22,22,22	1.82	3 (13%)	24,28,28	4.96	9 (37%)

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	NP	H	995	-	-	6/15/17/17	0/1/1/1
3	NP	B	996	-	-	10/15/17/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	996	NP	C5'-N5'	-6.40	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	995	NP	C5'-N5'	-5.48	1.35	1.45
3	H	995	NP	ON2-N5'	3.72	1.29	1.22
3	B	996	NP	ON2-N5'	3.23	1.28	1.22
3	B	996	NP	O4-C9	-2.22	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	995	NP	C1-C2-N3	30.42	158.28	116.06
3	H	995	NP	O2-C2-N3	-25.75	72.51	123.03
3	B	996	NP	O2-C2-C1	-19.62	79.46	121.99
3	H	995	NP	O2-C2-C1	-16.70	85.79	121.99
3	B	996	NP	C1-C2-N3	-7.48	105.68	116.06
3	B	996	NP	O2-C2-N3	-7.08	109.14	123.03
3	B	996	NP	C4-N3-C2	6.78	135.45	122.82
3	H	995	NP	C4-N3-C2	5.43	132.93	122.82
3	B	996	NP	C5-C4-N3	-4.24	100.30	112.20
3	H	995	NP	ON2-N5'-C5'	3.95	125.79	119.03
3	H	995	NP	O4-C9-C8	2.51	121.93	114.00
3	B	996	NP	C6-C5-C4	2.46	124.91	113.56
3	B	996	NP	C6'-C5'-C4'	-2.24	118.56	121.42
3	B	996	NP	ON2-N5'-C5'	2.22	122.83	119.03
3	B	996	NP	C5'-C6'-C1'	2.07	122.87	118.55
3	H	995	NP	C1'-C1-C2	-2.06	106.19	112.33
3	H	995	NP	O4'-C4'-C3'	-2.00	113.99	119.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	996	NP	C1-C2-N3-C4
3	B	996	NP	O2-C2-N3-C4
3	B	996	NP	C6-C7-C8-C9
3	H	995	NP	O2-C2-N3-C4
3	H	995	NP	C1'-C1-C2-O2
3	B	996	NP	C2-C1-C1'-C2'
3	B	996	NP	C2-C1-C1'-C6'
3	B	996	NP	C1'-C1-C2-O2
3	H	995	NP	C6-C7-C8-C9
3	H	995	NP	C5-C6-C7-C8
3	B	996	NP	C7-C8-C9-O3
3	H	995	NP	C7-C8-C9-O4

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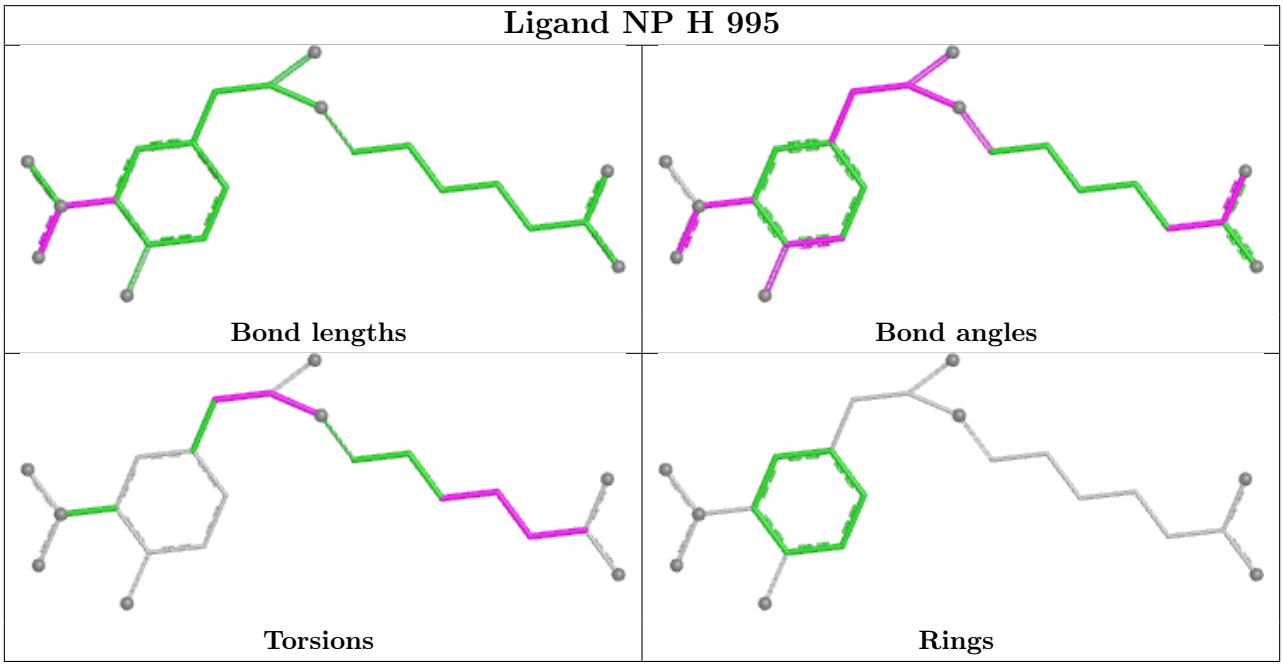
Mol	Chain	Res	Type	Atoms
3	B	996	NP	C7-C8-C9-O4
3	H	995	NP	C7-C8-C9-O3
3	B	996	NP	C5-C6-C7-C8
3	B	996	NP	C4-C5-C6-C7

There are no ring outliers.

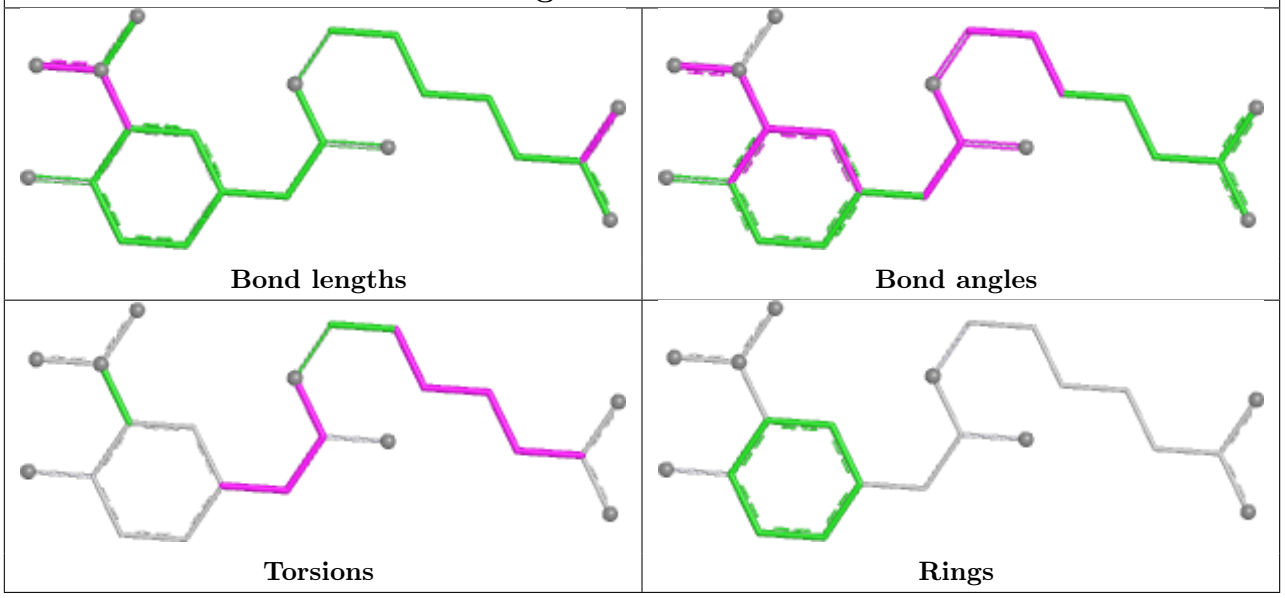
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	995	NP	1	0
3	B	996	NP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand NP B 996



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	H	1
1	A	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	117:SER	C	118:SER	N	3.13
1	H	117:SER	C	118:SER	N	3.12
1	A	109:LEU	C	110:GLY	N	3.02
1	L	109:LEU	C	110:GLY	N	2.88

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.