



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:18 AM UTC

PDB ID : 1A6V / pdb_00001a6v
Title : B1-8 FV fragment complexed with a (4-hydroxy-3-nitrophenyl) acetate compound
Authors : Simon, T.; Henrick, K.; Hirshberg, M.; Winter, G.
Deposited on : 1998-03-03
Resolution : 1.80 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

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**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

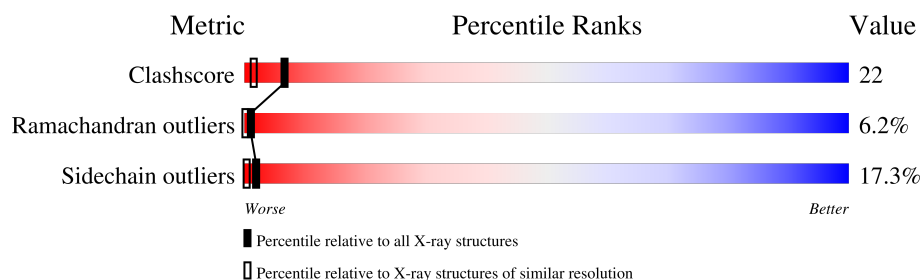
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	110	49% 43% 8%
1	M	110	56% 28% 13% ..
1	N	110	29% 41% 24% 5% .
2	H	120	39% 35% 19% 5% .
2	I	120	41% 45% 10% ..
2	J	120	22% 33% 35% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5798 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 B1-8 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	110	Total	C	N	O	S	0	0	0
			799	503	134	160	2			
1	M	109	Total	C	N	O	S	0	1	0
			814	513	139	160	2			
1	N	109	Total	C	N	O	S	0	0	0
			799	503	136	158	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	40	GLU	GLN	variant	UNP P01724
M	40	GLU	GLN	variant	UNP P01724
N	40	GLU	GLN	variant	UNP P01724

- Molecule 2 is a protein called B1-8 FV (HEAVY CHAIN).

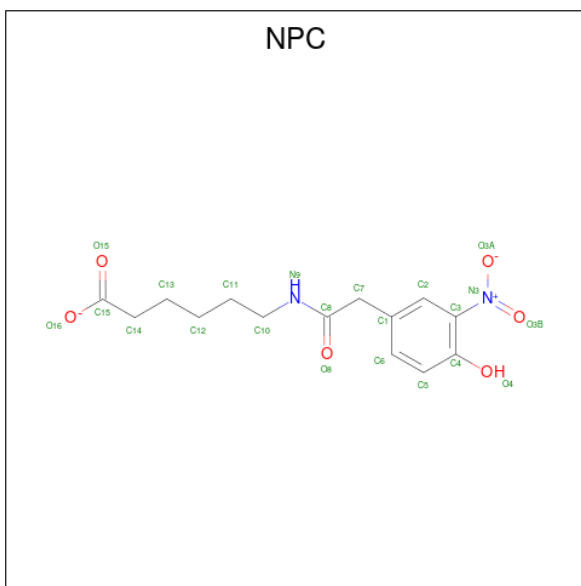
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	118	Total	C	N	O	S	0	1	0
			936	597	154	181	4			
2	I	119	Total	C	N	O	S	0	1	0
			942	600	155	183	4			
2	J	120	Total	C	N	O	S	0	1	0
			942	601	156	181	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	416	VAL	LEU	variant	UNP P01751
I	416	VAL	LEU	variant	UNP P01751
J	416	VAL	LEU	variant	UNP P01751

- Molecule 3 is 4-HYDROXY-3-NITROPHENYLACETYL-EPSILON-AMINOCAPROIC

ACID ANION (CCD ID: NPC) (formula: $C_{14}H_{17}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	1
			44	28	4	12		
3	I	1	Total	C	N	O	0	0
			22	14	2	6		
3	J	1	Total	C	N	O	0	0
			22	14	2	6		

- Molecule 4 is water.

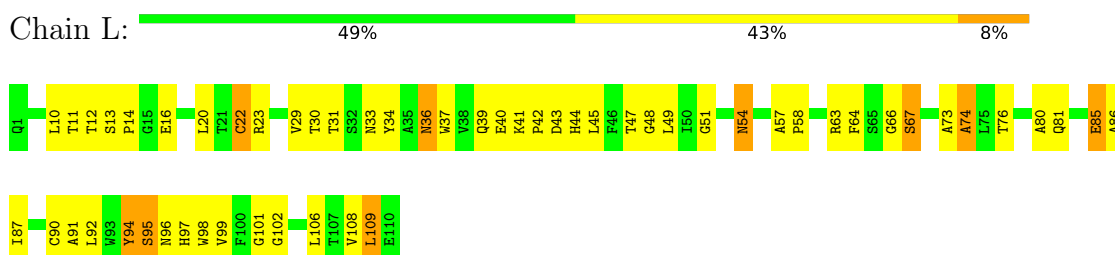
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	75	Total	O	0	0
			75	75		
4	H	81	Total	O	0	0
			81	81		
4	M	83	Total	O	0	0
			83	83		
4	I	86	Total	O	0	0
			86	86		
4	N	68	Total	O	0	0
			68	68		
4	J	85	Total	O	0	0
			85	85		

3 Residue-property plots [i](#)

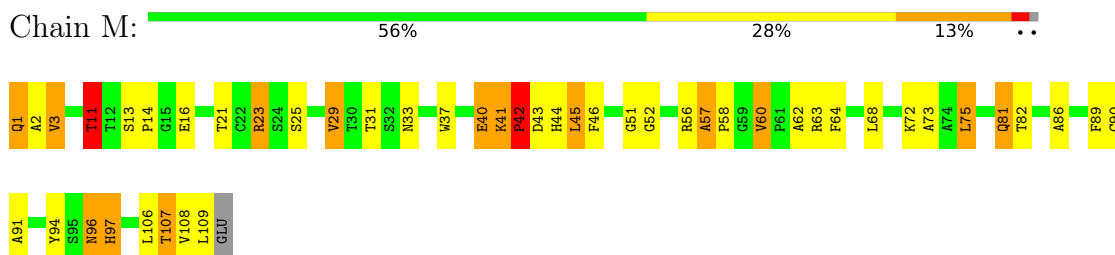
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

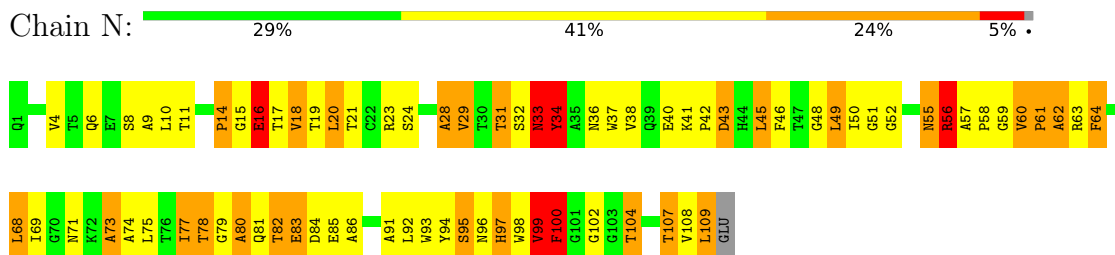
• Molecule 1: B1-8 FV (LIGHT CHAIN)



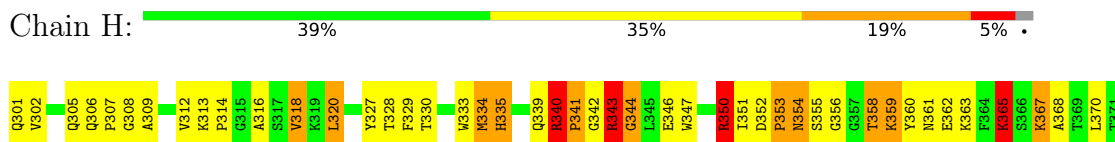
• Molecule 1: B1-8 FV (LIGHT CHAIN)

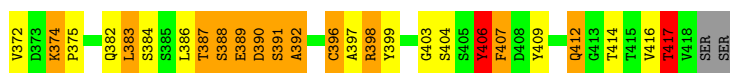


• Molecule 1: B1-8 FV (LIGHT CHAIN)



• Molecule 2: B1-8 FV (HEAVY CHAIN)

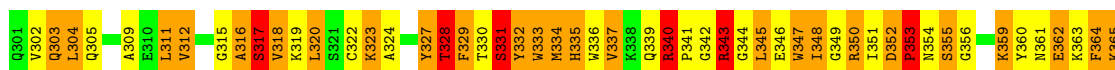
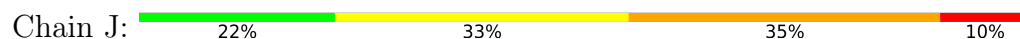




- Molecule 2: B1-8 FV (HEAVY CHAIN)



- Molecule 2: B1-8 FV (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	71.76Å 86.19Å 111.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.296 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5798	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NPC

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	1.12	0/817	2.42	48/1119 (4.3%)
1	M	1.14	0/837	2.39	43/1144 (3.8%)
1	N	1.13	2/816 (0.2%)	2.67	73/1115 (6.5%)
2	H	1.12	2/968 (0.2%)	2.56	74/1313 (5.6%)
2	I	1.02	0/974	2.23	43/1321 (3.3%)
2	J	1.13	2/974 (0.2%)	2.72	79/1320 (6.0%)
All	All	1.11	6/5386 (0.1%)	2.51	360/7332 (4.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	82	THR	C-O	9.21	1.35	1.24
1	N	82	THR	C-N	-5.33	1.25	1.33
2	J	418	VAL	C-N	-5.27	1.26	1.33
2	H	306	GLN	CD-OE1	5.18	1.33	1.23
2	J	419	SER	N-CA	-5.13	1.39	1.46
2	H	306	GLN	CD-NE2	-5.08	1.22	1.33

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	63	ARG	CD-NE-CZ	17.92	149.49	124.40
2	J	418	VAL	CA-C-N	16.39	152.84	121.54
2	J	418	VAL	C-N-CA	16.39	152.84	121.54
2	H	389	GLU	CA-C-N	15.59	151.32	121.54
2	H	389	GLU	C-N-CA	15.59	151.32	121.54
1	L	54	ASN	CA-CB-CG	12.52	125.12	112.60
1	L	64	PHE	CA-CB-CG	11.99	125.79	113.80
2	I	407	PHE	CA-CB-CG	11.87	125.67	113.80
2	H	359	LYS	CA-CB-CG	11.35	136.81	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	403	GLY	N-CA-C	10.96	139.14	113.18
2	J	398	ARG	NE-CZ-NH1	10.59	132.09	121.50
2	J	345	LEU	N-CA-C	10.53	126.07	110.48
2	J	398	ARG	CD-NE-CZ	10.52	139.13	124.40
2	H	389	GLU	CA-C-O	10.39	134.09	120.07
2	J	346	GLU	CA-CB-CG	9.79	133.68	114.10
1	L	43	ASP	CA-CB-CG	9.72	122.32	112.60
2	H	365	LYS	N-CA-C	9.70	121.44	111.07
2	J	345	LEU	CA-C-O	9.42	132.30	121.47
2	I	308	GLY	N-CA-C	9.32	124.70	112.77
1	N	29	VAL	N-CA-CB	9.26	123.34	111.67
1	N	55	ASN	CB-CA-C	9.23	124.94	109.80
2	H	344	GLY	CA-C-O	-9.21	110.08	119.20
2	J	309	ALA	N-CA-C	9.19	122.01	108.60
2	H	307	PRO	CA-C-N	9.06	130.00	119.94
2	H	307	PRO	C-N-CA	9.06	130.00	119.94
2	H	344	GLY	N-CA-C	9.05	126.91	115.42
1	N	31	THR	CB-CA-C	8.93	125.18	109.65
2	H	356	GLY	CA-C-N	8.89	129.37	120.31
2	H	356	GLY	C-N-CA	8.89	129.37	120.31
1	N	33	ASN	CA-CB-CG	8.88	121.48	112.60
1	M	56	ARG	CD-NE-CZ	8.88	136.83	124.40
1	L	76	THR	CA-CB-OG1	-8.80	96.41	109.60
1	M	81	GLN	CB-CG-CD	8.78	127.52	112.60
2	H	328	THR	CA-C-O	8.76	130.03	120.92
1	M	97	HIS	CA-CB-CG	8.70	122.50	113.80
1	N	63	ARG	NE-CZ-NH2	8.68	127.01	119.20
2	H	342	GLY	CA-C-N	8.68	138.11	121.54
2	H	342	GLY	C-N-CA	8.68	138.11	121.54
1	N	21	THR	CA-C-N	8.68	136.10	122.74
1	N	21	THR	C-N-CA	8.68	136.10	122.74
1	M	2	ALA	N-CA-C	-8.67	94.09	108.32
2	J	340	ARG	CD-NE-CZ	8.65	136.52	124.40
1	N	99	VAL	CB-CA-C	8.59	122.86	110.33
2	J	369	THR	N-CA-CB	8.57	124.98	110.49
1	N	82	THR	CA-C-O	-8.57	108.26	120.51
2	H	350	ARG	CA-CB-CG	8.56	131.22	114.10
2	I	408	ASP	CA-CB-CG	8.53	121.13	112.60
1	N	18	VAL	N-CA-CB	8.51	125.40	111.45
1	L	42	PRO	CA-C-N	8.44	137.66	121.54
1	L	42	PRO	C-N-CA	8.44	137.66	121.54
2	J	417	THR	CB-CA-C	8.43	125.39	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	343	ARG	N-CA-CB	8.40	124.69	110.49
1	M	56	ARG	CA-CB-CG	8.21	130.52	114.10
2	J	343	ARG	N-CA-C	-8.21	97.78	110.17
1	N	81	GLN	CA-C-N	8.13	137.08	121.54
1	N	81	GLN	C-N-CA	8.13	137.08	121.54
1	M	58	PRO	CB-CA-C	8.12	121.63	111.23
2	J	364	PHE	CA-C-O	-8.12	109.77	119.27
1	L	74	ALA	N-CA-C	8.11	121.79	109.23
2	J	355	SER	CA-C-N	8.08	137.25	121.41
2	J	355	SER	C-N-CA	8.08	137.25	121.41
2	H	389	GLU	N-CA-C	-8.06	102.21	112.93
1	N	96	ASN	N-CA-C	-8.04	104.07	114.04
2	I	389	GLU	CA-CB-CG	8.01	130.13	114.10
1	L	92	LEU	CA-C-O	8.00	129.20	120.32
1	N	97	HIS	CA-C-O	7.96	129.93	121.33
1	N	97	HIS	N-CA-C	7.95	121.16	109.07
1	M	45	LEU	CB-CA-C	7.92	124.83	111.22
1	N	17	THR	CA-C-O	-7.81	112.49	121.47
1	N	23	ARG	CA-C-O	7.80	128.97	120.32
1	N	23	ARG	CD-NE-CZ	7.76	135.26	124.40
2	I	396	CYS	N-CA-C	-7.75	97.12	109.59
2	H	404	SER	CA-C-N	7.68	133.97	122.68
2	H	404	SER	C-N-CA	7.68	133.97	122.68
2	J	320	LEU	CA-C-O	-7.62	112.35	120.80
2	H	356	GLY	N-CA-C	-7.59	105.34	115.21
2	J	371	THR	N-CA-CB	7.58	123.30	110.49
1	M	16	GLU	CA-CB-CG	7.56	129.22	114.10
2	J	410	TRP	CA-CB-CG	7.47	127.80	113.60
1	N	6	GLN	CA-C-O	-7.43	112.71	121.11
2	J	335	HIS	CA-CB-CG	7.39	121.19	113.80
2	H	352	ASP	CB-CA-C	7.36	117.83	110.33
2	J	355	SER	N-CA-C	7.33	126.41	110.80
2	H	343	ARG	NE-CZ-NH2	-7.33	112.61	119.20
1	M	1	GLN	CA-C-N	7.29	134.04	121.64
1	M	1	GLN	C-N-CA	7.29	134.04	121.64
1	N	34	TYR	CA-C-N	7.29	131.18	120.90
1	N	34	TYR	C-N-CA	7.29	131.18	120.90
1	N	97	HIS	CA-C-N	7.28	131.83	121.42
1	N	97	HIS	C-N-CA	7.28	131.83	121.42
2	J	340	ARG	N-CA-CB	7.27	120.11	110.29
2	I	326	GLY	N-CA-C	7.27	125.44	114.61
1	L	44	HIS	CA-CB-CG	7.25	121.05	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	320	LEU	CA-C-O	-7.23	113.05	120.71
2	I	358	THR	CA-CB-OG1	-7.21	98.78	109.60
1	N	20	LEU	CB-CA-C	7.21	122.91	109.71
2	J	398	ARG	NE-CZ-NH2	-7.21	112.71	119.20
2	J	333	TRP	CB-CA-C	7.20	122.10	110.29
1	L	22	CYS	CA-C-N	7.19	133.36	122.93
1	L	22	CYS	C-N-CA	7.19	133.36	122.93
2	J	352	ASP	O-C-N	7.18	130.19	121.29
1	N	4	VAL	CB-CA-C	7.14	120.56	110.84
1	L	43	ASP	CA-C-N	7.11	135.12	121.54
1	L	43	ASP	C-N-CA	7.11	135.12	121.54
2	H	343	ARG	CA-CB-CG	7.06	128.22	114.10
2	J	352	ASP	N-CA-CB	7.01	122.61	110.05
1	L	36	ASN	CA-C-O	-6.98	112.82	120.36
2	I	354	ASN	CB-CG-ND2	-6.95	105.97	116.40
1	L	96	ASN	CA-CB-CG	6.91	119.51	112.60
2	J	380	TYR	N-CA-C	6.83	120.08	107.99
2	J	320	LEU	CB-CA-C	6.83	120.95	109.48
2	H	308	GLY	N-CA-C	6.82	120.41	112.50
2	J	383	LEU	CA-C-O	-6.81	112.84	120.54
2	H	333	TRP	CB-CA-C	6.78	121.11	109.51
1	N	63	ARG	NE-CZ-NH1	-6.78	114.72	121.50
2	H	352	ASP	CA-CB-CG	6.74	119.34	112.60
2	J	383	LEU	O-C-N	6.73	130.89	123.22
2	J	349	GLY	CA-C-O	-6.72	115.73	121.04
1	M	29	VAL	CA-C-O	-6.68	114.08	121.23
2	H	346	GLU	N-CA-CB	6.66	121.86	110.68
2	J	383	LEU	N-CA-C	-6.66	98.41	109.46
1	L	99	VAL	N-CA-CB	6.65	121.23	111.52
1	L	94	TYR	N-CA-CB	6.60	120.91	110.55
2	J	401	TYR	CA-C-N	6.60	133.17	122.81
2	J	401	TYR	C-N-CA	6.60	133.17	122.81
2	H	367	LYS	CA-C-N	6.60	130.85	121.42
2	H	367	LYS	C-N-CA	6.60	130.85	121.42
2	J	328	THR	CA-C-N	6.59	134.12	121.54
2	J	328	THR	C-N-CA	6.59	134.12	121.54
2	J	378	THR	CA-CB-CG2	6.58	121.68	110.50
2	I	415	THR	CA-CB-CG2	6.56	121.64	110.50
2	J	334	MET	N-CA-C	-6.47	99.47	109.76
1	M	63	ARG	CA-C-N	6.46	131.92	123.00
1	M	63	ARG	C-N-CA	6.46	131.92	123.00
2	H	387	THR	CA-C-N	6.46	133.87	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	387	THR	C-N-CA	6.46	133.87	121.54
2	H	399	TYR	CA-C-O	6.44	128.06	120.20
1	M	52	GLY	O-C-N	-6.44	117.30	122.51
1	M	23	ARG	CA-CB-CG	6.43	126.97	114.10
2	J	303	GLN	OE1-CD-NE2	-6.43	116.17	122.60
2	H	387	THR	CB-CA-C	6.40	121.42	110.79
2	J	395	TYR	CA-CB-CG	6.40	125.42	113.90
1	M	44	HIS	CA-CB-CG	6.38	120.18	113.80
2	H	361	ASN	CA-CB-CG	6.37	118.97	112.60
1	N	104	THR	CA-C-O	-6.34	113.46	120.38
2	J	368	ALA	CA-C-N	6.34	133.65	121.54
2	J	368	ALA	C-N-CA	6.34	133.65	121.54
2	H	406	TYR	CA-CB-CG	6.34	125.31	113.90
2	J	337	VAL	CA-C-N	6.33	132.08	122.65
2	J	337	VAL	C-N-CA	6.33	132.08	122.65
1	L	63	ARG	NE-CZ-NH2	-6.32	113.51	119.20
2	J	349	GLY	O-C-N	6.32	129.04	123.80
2	I	345	LEU	CA-C-O	6.31	128.94	121.36
1	M	60	VAL	O-C-N	6.31	128.83	121.57
2	J	311	LEU	CA-C-O	-6.30	113.53	120.33
1	L	13	SER	O-C-N	6.30	126.35	121.88
1	N	40	GLU	CA-C-O	6.29	127.03	120.30
1	M	43	ASP	CA-CB-CG	6.29	118.89	112.60
2	J	328	THR	CA-C-O	6.29	129.50	120.51
1	N	21	THR	CA-C-O	6.28	129.16	121.56
2	J	366	SER	N-CA-CB	-6.26	100.91	111.17
2	H	361	ASN	CA-C-O	-6.25	113.33	120.58
2	I	392	ALA	CA-C-O	-6.23	114.46	121.25
1	L	54	ASN	N-CA-C	6.20	120.47	112.41
1	M	44	HIS	CA-C-O	6.20	129.38	120.51
2	J	327	TYR	CA-CB-CG	6.18	125.03	113.90
1	N	64	PHE	CA-C-O	-6.18	113.32	120.49
1	M	57	ALA	N-CA-C	-6.18	102.00	109.72
1	N	60	VAL	O-C-N	6.17	128.13	121.10
2	I	390	ASP	N-CA-CB	6.16	119.71	110.65
2	J	362	GLU	CA-C-N	6.15	128.85	120.54
2	J	362	GLU	C-N-CA	6.15	128.85	120.54
1	L	36	ASN	CA-CB-CG	6.15	118.75	112.60
1	L	96	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	M	81	GLN	CA-CB-CG	6.11	126.32	114.10
2	H	318	VAL	CA-CB-CG1	6.10	120.77	110.40
1	L	34	TYR	CB-CA-C	6.06	120.95	112.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	314	PRO	CB-CA-C	6.01	119.08	111.39
1	M	40	GLU	CB-CG-CD	5.97	122.75	112.60
2	I	354	ASN	N-CA-C	5.97	117.87	111.36
2	H	305	GLN	CA-C-O	5.97	126.75	120.36
2	H	354	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	N	56	ARG	N-CA-C	5.97	119.46	107.41
2	H	361	ASN	N-CA-C	-5.96	100.82	109.59
2	I	334	MET	CA-C-O	5.96	126.56	120.24
2	J	322	CYS	CA-CB-SG	5.95	128.08	114.40
1	L	44	HIS	CA-C-N	5.95	130.33	122.30
1	L	44	HIS	C-N-CA	5.95	130.33	122.30
1	N	4	VAL	CA-CB-CG1	5.94	120.50	110.40
2	J	332	TYR	CA-C-N	-5.94	113.11	121.72
2	J	332	TYR	C-N-CA	-5.94	113.11	121.72
1	N	11	THR	CB-CA-C	5.94	119.29	110.62
1	L	58	PRO	CB-CA-C	5.93	119.12	111.46
1	M	90	CYS	N-CA-CB	5.93	120.34	110.85
1	N	108	VAL	N-CA-CB	5.92	118.92	111.46
2	H	355	SER	N-CA-C	5.92	117.41	111.07
1	N	94	TYR	CA-C-N	5.92	132.84	121.54
1	N	94	TYR	C-N-CA	5.92	132.84	121.54
1	N	45	LEU	CA-C-N	5.92	130.53	122.84
1	N	45	LEU	C-N-CA	5.92	130.53	122.84
2	J	367[A]	LYS	N-CA-C	-5.91	105.07	112.93
2	J	367[B]	LYS	N-CA-C	-5.91	105.07	112.93
1	N	104	THR	O-C-N	5.89	130.24	123.29
2	H	388	SER	N-CA-CB	5.88	120.43	110.49
2	J	348	ILE	N-CA-C	-5.88	106.75	111.81
1	L	29	VAL	N-CA-C	-5.87	100.02	108.53
1	M	91	ALA	N-CA-CB	-5.86	100.67	110.80
1	N	19	THR	O-C-N	5.85	130.26	123.30
2	H	350	ARG	CB-CG-CD	5.84	124.74	111.30
2	H	396	CYS	N-CA-C	-5.84	99.88	109.40
2	J	419	SER	O-C-N	5.83	130.35	122.59
2	H	350	ARG	CG-CD-NE	5.80	124.77	112.00
2	J	390	ASP	CA-CB-CG	-5.79	106.81	112.60
2	H	407	PHE	CA-CB-CG	5.79	119.59	113.80
1	L	87	ILE	N-CA-CB	5.79	118.75	111.46
2	I	392	ALA	O-C-N	5.78	129.05	123.04
1	N	61	PRO	CA-C-O	-5.78	115.05	121.23
2	H	359	LYS	N-CA-CB	5.76	119.89	110.90
2	H	340	ARG	N-CA-CB	5.75	120.61	110.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	31	THR	CA-CB-CG2	5.75	120.28	110.50
2	H	335	HIS	CA-C-O	-5.74	114.50	120.70
2	J	345	LEU	N-CA-CB	-5.74	101.57	110.29
2	I	345	LEU	N-CA-C	5.72	119.41	110.32
1	N	77	ILE	CA-C-O	-5.71	113.98	120.66
1	L	96	ASN	N-CA-C	5.69	119.21	112.72
1	N	29	VAL	CA-CB-CG2	5.69	120.07	110.40
1	L	43	ASP	CA-C-O	5.68	128.63	120.51
1	N	109	LEU	CB-CA-C	5.67	120.88	110.10
2	I	413	GLY	CA-C-O	5.67	127.17	122.24
2	J	334	MET	CA-C-O	-5.67	114.23	120.69
1	N	49	LEU	N-CA-C	5.67	120.69	113.55
2	H	392	ALA	N-CA-CB	-5.66	102.30	111.24
1	N	64	PHE	O-C-N	5.66	129.98	123.02
1	N	85	GLU	CB-CG-CD	5.65	122.21	112.60
2	H	309	ALA	N-CA-C	5.59	116.46	108.74
2	H	344	GLY	CA-C-N	-5.59	114.99	122.42
2	H	344	GLY	C-N-CA	-5.59	114.99	122.42
2	I	358	THR	N-CA-C	5.59	118.57	109.24
1	M	16	GLU	CB-CG-CD	5.57	122.06	112.60
2	J	353	PRO	CB-CA-C	5.56	120.73	111.56
1	M	46	PHE	CA-CB-CG	5.55	119.35	113.80
1	L	67	SER	CA-CB-OG	5.55	122.20	111.10
1	L	45	LEU	N-CA-C	5.54	117.76	108.96
2	H	358	THR	CA-C-N	5.54	130.47	122.44
2	H	358	THR	C-N-CA	5.54	130.47	122.44
2	J	362	GLU	CB-CG-CD	5.54	122.01	112.60
2	I	333	TRP	N-CA-CB	-5.52	101.63	110.46
2	I	328	THR	N-CA-CB	5.50	118.22	110.24
2	H	398	ARG	O-C-N	5.49	129.46	123.04
1	L	34	TYR	CA-CB-CG	-5.49	104.02	113.90
1	L	101	GLY	N-CA-C	-5.49	104.02	112.85
2	H	328	THR	O-C-N	-5.48	115.72	122.68
2	I	358	THR	CA-CB-CG2	5.48	119.81	110.50
2	H	359	LYS	CB-CA-C	-5.48	102.62	110.62
2	I	367	LYS	O-C-N	5.47	127.83	122.19
1	N	23	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	N	28	ALA	CA-C-N	-5.47	115.67	123.11
1	N	28	ALA	C-N-CA	-5.47	115.67	123.11
2	I	403	GLY	CA-C-N	5.45	129.41	120.63
2	I	403	GLY	C-N-CA	5.45	129.41	120.63
1	M	33	ASN	CB-CG-ND2	5.45	124.58	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	97	HIS	CA-C-O	5.45	127.11	121.28
1	M	3	VAL	N-CA-CB	-5.44	105.57	112.15
1	N	55	ASN	CA-CB-CG	5.44	118.04	112.60
1	N	96	ASN	O-C-N	5.43	128.77	122.25
2	H	358	THR	CA-CB-OG1	-5.42	101.46	109.60
1	N	84	ASP	CA-CB-CG	5.42	118.02	112.60
1	M	107	THR	CA-C-O	-5.42	114.56	120.36
1	L	106	LEU	O-C-N	5.41	129.95	123.13
2	J	418	VAL	CA-C-O	5.40	127.53	120.78
2	H	362	GLU	CB-CG-CD	5.40	121.78	112.60
2	J	317	SER	N-CA-C	5.39	122.29	110.80
2	J	402	TYR	N-CA-C	-5.39	101.09	109.72
2	I	390	ASP	N-CA-C	-5.39	106.72	113.72
1	L	43	ASP	CB-CA-C	5.38	121.13	110.42
1	N	74	ALA	CA-C-N	5.38	130.36	122.39
1	N	74	ALA	C-N-CA	5.38	130.36	122.39
2	J	319	LYS	N-CA-C	-5.38	99.00	108.20
1	M	52	GLY	CA-C-N	5.38	131.81	121.54
1	M	52	GLY	C-N-CA	5.38	131.81	121.54
2	J	375	PRO	CA-C-O	5.38	126.53	119.00
2	I	303	GLN	CB-CA-C	5.37	118.93	109.80
2	I	404	SER	N-CA-C	5.37	119.32	112.34
2	I	408	ASP	N-CA-C	5.37	117.95	111.40
1	N	100	PHE	CA-C-N	5.36	126.58	120.53
1	N	100	PHE	C-N-CA	5.36	126.58	120.53
1	M	60	VAL	CA-C-O	-5.35	115.09	119.47
1	N	107	THR	CA-CB-CG2	5.33	119.56	110.50
2	J	337	VAL	CA-C-O	5.33	128.35	121.32
2	J	383	LEU	N-CA-CB	5.31	118.93	110.16
1	L	54	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	N	31	THR	O-C-N	-5.30	115.48	122.42
1	M	89	PHE	CA-CB-CG	5.29	119.09	113.80
2	I	354	ASN	CB-CA-C	-5.29	101.85	110.85
2	I	370	LEU	CA-C-O	5.29	126.31	120.71
2	I	415	THR	CA-C-O	-5.28	115.28	120.98
2	J	316	ALA	CA-C-N	5.27	131.60	121.54
2	J	316	ALA	C-N-CA	5.27	131.60	121.54
2	I	333	TRP	CB-CA-C	5.25	119.01	109.83
1	L	91	ALA	O-C-N	5.24	129.25	123.33
2	J	343	ARG	N-CA-CB	5.24	118.94	110.51
2	H	309	ALA	CA-C-O	5.23	126.91	121.36
1	M	58	PRO	CA-C-O	5.23	127.63	121.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	363	LYS	N-CA-C	5.23	119.14	112.34
2	H	417	THR	CA-C-O	-5.23	114.86	120.46
1	N	19	THR	CA-CB-OG1	-5.22	101.76	109.60
2	J	347	TRP	CA-C-N	-5.21	116.21	122.35
2	J	347	TRP	C-N-CA	-5.21	116.21	122.35
2	I	367	LYS	CA-CB-CG	5.20	124.49	114.10
1	N	73	ALA	N-CA-C	-5.19	100.72	109.07
1	L	48	GLY	CA-C-O	-5.18	116.91	121.58
1	N	78	THR	N-CA-C	5.18	119.59	113.16
1	L	23	ARG	N-CA-C	5.17	117.91	109.59
1	L	16	GLU	CA-CB-CG	5.17	124.44	114.10
1	M	106	LEU	N-CA-C	-5.17	100.10	108.52
1	L	57	ALA	N-CA-C	-5.17	103.52	109.93
2	I	388	SER	N-CA-C	-5.16	106.49	112.89
2	H	383	LEU	CB-CA-C	5.16	118.39	110.14
2	J	402	TYR	N-CA-CB	5.15	119.89	111.08
2	H	365	LYS	CG-CD-CE	5.15	123.14	111.30
1	L	97	HIS	CA-CB-CG	-5.14	108.66	113.80
1	M	21	THR	CA-C-N	5.13	130.17	122.47
1	M	21	THR	C-N-CA	5.13	130.17	122.47
1	N	34	TYR	CA-CB-CG	5.13	123.14	113.90
1	N	16	GLU	O-C-N	5.12	129.11	122.81
1	M	64	PHE	CA-C-O	5.12	125.96	120.38
2	J	343	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	N	108	VAL	CA-C-N	-5.10	112.51	121.70
1	N	108	VAL	C-N-CA	-5.10	112.51	121.70
2	H	334	MET	CG-SD-CE	5.10	112.12	100.90
1	L	45	LEU	CA-C-O	-5.10	114.72	120.43
1	M	40	GLU	N-CA-CB	5.10	118.71	110.65
1	L	91	ALA	CA-C-N	5.09	130.58	122.74
1	L	91	ALA	C-N-CA	5.09	130.58	122.74
2	I	385	SER	N-CA-CB	-5.09	104.34	111.62
2	I	406	TYR	CA-CB-CG	5.09	123.07	113.90
1	N	34	TYR	CA-C-O	5.09	127.78	120.51
2	J	343	ARG	CA-CB-CG	5.08	124.27	114.10
1	L	98	TRP	N-CA-C	-5.08	101.99	110.17
1	M	81	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	N	40	GLU	CG-CD-OE1	5.08	130.09	118.40
2	H	383	LEU	CA-C-O	-5.08	114.86	120.24
2	I	380	TYR	N-CA-C	5.07	117.60	110.14
1	N	59	GLY	CA-C-N	5.07	131.51	122.13
1	N	59	GLY	C-N-CA	5.07	131.51	122.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	372	VAL	CA-CB-CG2	5.07	119.01	110.40
2	I	407	PHE	N-CA-C	-5.06	99.08	108.24
2	J	405	SER	N-CA-CB	-5.06	101.94	110.49
2	H	316	ALA	N-CA-C	5.04	116.85	108.02
2	H	362	GLU	CG-CD-OE1	5.04	129.99	118.40
1	L	29	VAL	CB-CA-C	5.04	118.47	110.81
2	H	409	TYR	CB-CA-C	5.04	118.06	109.80
2	J	408	ASP	N-CA-C	5.03	117.16	111.02
1	M	11	THR	CA-CB-CG2	5.03	119.04	110.50
1	N	83	GLU	CG-CD-OE1	5.03	129.96	118.40
2	H	343	ARG	N-CA-C	-5.02	100.10	110.80
2	I	407	PHE	N-CA-CB	5.02	117.87	110.49
2	I	315	GLY	CA-C-N	5.02	132.12	122.03
2	I	315	GLY	C-N-CA	5.02	132.12	122.03
2	I	324	ALA	N-CA-CB	-5.01	102.24	110.41

There are no chirality outliers.

There are no planarity outliers.

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	799	0	756	20	0
1	M	814	0	796	18	0
1	N	799	0	769	45	0
2	H	936	0	893	43	0
2	I	942	0	899	38	0
2	J	942	0	891	76	0
3	H	44	0	34	3	0
3	I	22	0	17	3	0
3	J	22	0	17	1	0
4	H	81	0	0	6	0
4	I	86	0	0	3	0
4	J	85	0	0	7	0
4	L	75	0	0	0	0
4	M	83	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	68	0	0	8	0
All	All	5798	0	5072	225	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 22.

All (225) 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:J:323:LYS:HA	2:J:378:THR:HB	1.60	0.82
2:J:353:PRO:HA	2:J:372:VAL:HG11	1.61	0.81
3:H:430[A]:NPC:O15	3:H:430[A]:NPC:H122	1.80	0.81
2:I:335:HIS:HD2	2:I:347:TRP:HE1	1.29	0.78
2:J:304:LEU:HD13	2:J:334:MET:HE1	1.65	0.77
1:N:56:ARG:HE	1:N:62:ALA:HA	1.47	0.76
1:L:51:GLY:HA3	2:H:406:TYR:HB3	1.65	0.76
1:M:51:GLY:HA3	2:I:406:TYR:HB3	1.68	0.75
2:H:412:GLN:H	2:H:412:GLN:HE21	1.34	0.75
1:N:34:TYR:HB3	1:N:52:GLY:HA2	1.67	0.74
2:J:347:TRP:HB3	2:J:361:ASN:HD22	1.51	0.74
1:N:31:THR:HB	1:N:34:TYR:CE1	2.24	0.72
2:H:350:ARG:HE	2:H:359:LYS:HG2	1.55	0.70
2:J:302:VAL:HG13	2:J:327:TYR:HB3	1.72	0.69
1:N:24:SER:HB2	1:N:29:VAL:HG13	1.74	0.69
2:J:351:ILE:HB	2:J:370:LEU:HD12	1.74	0.69
2:H:334:MET:HE2	2:H:396:CYS:HB2	1.74	0.68
2:J:330:THR:O	2:J:331:SER:HB3	1.94	0.68
2:H:335:HIS:HD2	2:H:347:TRP:HE1	1.42	0.68
3:I:430:NPC:H6	3:I:430:NPC:H101	1.75	0.68
2:H:350:ARG:HG3	3:H:430[A]:NPC:O3B	1.94	0.68
2:I:334:MET:HB3	2:I:351:ILE:HG22	1.75	0.67
2:J:318:VAL:HG22	2:J:386:LEU:HD11	1.77	0.67
2:I:339:GLN:HB2	2:I:345:LEU:HD23	1.75	0.67
2:I:335:HIS:CD2	2:I:347:TRP:HE1	2.10	0.66
1:N:56:ARG:HB3	1:N:56:ARG:HH11	1.59	0.66
1:L:85:GLU:HG3	1:L:108:VAL:H	1.61	0.66
2:J:354:ASN:HA	2:J:374:LYS:HE3	1.77	0.65
1:N:20:LEU:HD23	1:N:104:THR:HG21	1.78	0.65
2:I:330:THR:HA	2:I:353:PRO:HB2	1.78	0.65
2:I:354:ASN:HD21	2:J:341:PRO:HG2	1.61	0.64
2:H:360:TYR:HB2	2:H:365:LYS:HD2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:92:LEU:HB2	1:N:99:VAL:HG22	1.79	0.64
1:N:46:PHE:HE2	2:J:345:LEU:HD11	1.63	0.64
1:N:57:ALA:HB2	2:J:406:TYR:HB2	1.79	0.64
1:L:102:GLY:HA2	2:H:343:ARG:HB3	1.80	0.63
2:I:340:ARG:HB3	2:I:341:PRO:HD2	1.80	0.63
2:H:343:ARG:HD2	2:H:344:GLY:H	1.65	0.62
2:J:351:ILE:HD13	2:J:379:ALA:HB1	1.81	0.62
2:H:330:THR:HB	2:H:354:ASN:HD21	1.65	0.62
1:M:29:VAL:HG11	1:M:73:ALA:HB2	1.81	0.62
2:H:335:HIS:CD2	2:H:347:TRP:HE1	2.18	0.61
2:I:374:LYS:HG2	2:I:375:PRO:HD3	1.81	0.61
2:J:370:LEU:HD22	2:J:381:MET:HG2	1.81	0.61
2:J:352:ASP:HA	4:J:478:HOH:O	2.01	0.60
1:M:82:THR:HA	1:M:108:VAL:HB	1.82	0.60
1:N:36:ASN:HD21	2:J:399:TYR:HE2	1.48	0.60
2:H:320:LEU:HD22	2:H:414:THR:HG21	1.83	0.59
2:J:312:VAL:C	2:J:419:SER:HB3	2.27	0.59
1:L:10:LEU:HD12	1:L:20:LEU:HG	1.83	0.59
2:I:350:ARG:HH21	2:I:359:LYS:HE3	1.67	0.59
1:N:24:SER:HB2	1:N:29:VAL:CG1	2.34	0.58
1:M:82:THR:HG22	1:M:108:VAL:O	2.04	0.58
2:J:328:THR:O	2:J:329:PHE:HB2	2.04	0.57
2:I:318:VAL:HG22	2:I:386:LEU:HD11	1.87	0.57
1:N:29:VAL:HG23	1:N:68:LEU:HD22	1.85	0.57
2:H:391:SER:HA	2:H:416:VAL:O	2.05	0.57
1:N:38:VAL:HA	1:N:48:GLY:HA2	1.87	0.56
2:J:374:LYS:HB2	2:J:375:PRO:HD3	1.87	0.56
2:J:351:ILE:HD12	2:J:371:THR:H	1.70	0.56
2:H:350:ARG:NE	2:H:359:LYS:HG2	2.21	0.56
1:N:102:GLY:HA2	2:J:343:ARG:HH12	1.70	0.56
2:H:350:ARG:HH21	2:H:359:LYS:HD3	1.71	0.55
1:M:94:TYR:HB2	1:M:97:HIS:CD2	2.41	0.55
1:N:28:ALA:HA	1:N:71:ASN:HB2	1.89	0.55
2:H:412:GLN:H	2:H:412:GLN:NE2	2.03	0.55
1:N:46:PHE:CE2	2:J:345:LEU:HD11	2.42	0.55
2:J:302:VAL:HG21	2:J:398:ARG:NH1	2.22	0.55
1:L:39:GLN:HB2	1:L:49:LEU:HD11	1.89	0.55
2:H:358:THR:HG21	2:H:370:LEU:HB2	1.87	0.54
1:N:29:VAL:HG21	1:N:73:ALA:HB2	1.88	0.54
1:N:37:TRP:HB2	1:N:50:ILE:HB	1.89	0.54
2:H:330:THR:HB	2:H:354:ASN:ND2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:339:GLN:O	2:H:392:ALA:HB1	2.07	0.54
1:L:41:LYS:HD2	1:L:86:ALA:HB2	1.89	0.53
1:L:81:GLN:O	1:L:108:VAL:HG21	2.08	0.53
1:L:102:GLY:O	2:H:343:ARG:HB3	2.08	0.53
2:J:333:TRP:HA	4:J:479:HOH:O	2.07	0.53
2:I:350:ARG:NH2	2:I:359:LYS:HB2	2.23	0.52
1:N:73:ALA:HB3	4:N:379:HOH:O	2.09	0.52
1:N:64:PHE:CD2	1:N:77:ILE:HD11	2.44	0.52
2:H:350:ARG:HD2	2:H:350:ARG:C	2.34	0.51
1:N:41:LYS:HB3	1:N:42:PRO:HD2	1.91	0.51
2:H:350:ARG:HD2	2:H:351:ILE:N	2.26	0.51
2:H:341:PRO:HA	4:H:111:HOH:O	2.09	0.51
2:I:387:THR:HG23	2:I:389:GLU:HB3	1.93	0.50
2:J:341:PRO:C	2:J:343:ARG:H	2.17	0.50
2:H:350:ARG:HH21	2:H:359:LYS:CD	2.25	0.50
1:M:81:GLN:C	1:M:108:VAL:HG11	2.36	0.50
2:I:333:TRP:CE3	2:I:350:ARG:HD3	2.47	0.50
1:N:49:LEU:HA	1:N:60:VAL:HG21	1.92	0.49
2:J:340:ARG:HG3	2:J:340:ARG:HH11	1.76	0.49
1:L:14:PRO:HA	1:L:80:ALA:O	2.12	0.49
1:M:94:TYR:HB2	1:M:97:HIS:HD2	1.77	0.49
2:I:339:GLN:HB2	2:I:345:LEU:CD2	2.43	0.49
2:I:323:LYS:HG3	2:I:378:THR:OG1	2.12	0.49
1:N:97:HIS:HA	4:N:385:HOH:O	2.13	0.48
2:I:301:GLN:HA	4:I:439:HOH:O	2.12	0.48
2:H:368:ALA:HA	2:H:382:GLN:O	2.14	0.48
2:H:374:LYS:NZ	2:I:419:SER:HA	2.28	0.48
1:M:11:THR:HB	1:M:107:THR:HB	1.94	0.48
1:N:109:LEU:HD13	1:N:109:LEU:C	2.39	0.48
1:N:16:GLU:HB2	4:N:334:HOH:O	2.13	0.47
2:J:351:ILE:HD11	2:J:372:VAL:HG13	1.95	0.47
2:H:390:ASP:O	2:H:392:ALA:N	2.47	0.47
1:N:15:GLY:O	1:N:79:GLY:HA2	2.14	0.47
2:H:320:LEU:HG	4:H:91:HOH:O	2.14	0.47
1:M:41:LYS:HB3	1:M:42:PRO:HD2	1.95	0.47
2:I:391:SER:HA	2:I:416:VAL:O	2.15	0.47
1:N:14:PRO:HA	1:N:80:ALA:O	2.13	0.47
1:L:22:CYS:HB3	1:L:73:ALA:HB3	1.96	0.47
1:L:81:GLN:C	1:L:108:VAL:HG21	2.40	0.46
2:J:335:HIS:CE1	2:J:350:ARG:HB3	2.49	0.46
2:H:302:VAL:HG13	2:H:327:TYR:CD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:12:THR:HG23	1:L:108:VAL:HA	1.97	0.46
1:M:13:SER:O	1:M:14:PRO:C	2.57	0.46
1:N:51:GLY:O	1:N:52:GLY:C	2.58	0.46
2:I:350:ARG:HH21	2:I:359:LYS:HB2	1.80	0.46
2:J:361:ASN:HB3	2:J:364:PHE:HD2	1.81	0.46
2:J:371:THR:O	2:J:380:TYR:HB2	2.16	0.46
2:J:384:SER:O	2:J:386:LEU:HG	2.16	0.46
1:M:3:VAL:HB	1:M:25:SER:HB3	1.98	0.46
1:N:9:ALA:HB1	4:N:390:HOH:O	2.15	0.46
2:J:302:VAL:HG21	2:J:398:ARG:HH11	1.79	0.46
2:I:404:SER:O	2:I:405:SER:HB2	2.16	0.46
2:J:331:SER:OG	2:J:332:TYR:N	2.49	0.46
2:I:350:ARG:NH2	2:I:359:LYS:HE3	2.32	0.45
2:J:397:ALA:HA	2:J:410:TRP:HA	1.98	0.45
1:L:14:PRO:HD3	1:L:109:LEU:HA	1.98	0.45
2:J:391:SER:HA	2:J:416:VAL:O	2.17	0.45
1:M:23:ARG:NH1	1:M:72:LYS:NZ	2.64	0.45
2:J:303:GLN:HG2	2:J:305:GLN:HG2	1.99	0.45
2:J:329:PHE:O	2:J:353:PRO:HB2	2.17	0.45
2:J:330:THR:HB	4:J:463:HOH:O	2.17	0.44
2:H:374:LYS:N	2:H:375:PRO:CD	2.80	0.44
2:J:364:PHE:HA	2:J:367[A]:LYS:HB2	1.99	0.44
2:J:399:TYR:HA	2:J:406:TYR:O	2.18	0.44
2:J:412:GLN:HB2	4:J:509:HOH:O	2.17	0.44
2:H:351:ILE:O	2:H:353:PRO:HD3	2.18	0.44
2:I:354:ASN:HD21	2:J:341:PRO:CG	2.28	0.44
2:J:311:LEU:O	2:J:312:VAL:HB	2.16	0.44
2:J:317:SER:HA	2:J:384:SER:O	2.17	0.44
1:N:56:ARG:NE	1:N:62:ALA:HA	2.24	0.44
1:N:64:PHE:CE2	1:N:77:ILE:HD11	2.52	0.44
1:N:91:ALA:HB2	1:N:100:PHE:CZ	2.53	0.44
2:H:334:MET:HE2	2:H:396:CYS:CB	2.44	0.44
1:M:1:GLN:HG3	4:M:116:HOH:O	2.18	0.44
1:M:37:TRP:CE3	1:M:75:LEU:HD23	2.53	0.44
2:I:352:ASP:N	2:I:357:GLY:O	2.50	0.44
2:I:311:LEU:HA	2:I:417:THR:HG23	1.99	0.44
1:N:50:ILE:HA	1:N:55:ASN:O	2.18	0.44
2:H:334:MET:HE3	2:H:397:ALA:N	2.32	0.43
1:M:81:GLN:HG3	4:M:182:HOH:O	2.17	0.43
1:L:12:THR:CG2	1:L:108:VAL:HA	2.48	0.43
1:M:40:GLU:O	1:M:86:ALA:HB1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:330:THR:O	2:I:354:ASN:ND2	2.50	0.43
2:I:361:ASN:HB3	2:I:364:PHE:HD2	1.83	0.43
2:I:402:TYR:HB3	2:J:342:GLY:HA3	2.01	0.43
2:J:324:ALA:HB1	2:J:327:TYR:CE1	2.53	0.43
2:J:351:ILE:CB	2:J:370:LEU:HD12	2.44	0.43
2:H:398:ARG:O	2:H:407:PHE:HA	2.19	0.43
1:N:41:LYS:CB	1:N:42:PRO:HD2	2.49	0.43
2:H:417:THR:HG21	4:H:153:HOH:O	2.17	0.43
2:I:401:TYR:CE1	3:I:430:NPC:H121	2.54	0.43
2:I:399:TYR:HA	2:I:406:TYR:O	2.19	0.43
2:J:381:MET:HE1	2:J:383:LEU:HD23	2.00	0.43
1:L:66:GLY:HA2	1:L:74:ALA:O	2.19	0.43
2:I:402:TYR:CD1	2:J:342:GLY:HA3	2.53	0.43
2:I:368:ALA:HA	2:I:382:GLN:O	2.19	0.42
2:H:365:LYS:C	2:H:367:LYS:H	2.27	0.42
1:M:57:ALA:O	1:M:60:VAL:HG23	2.19	0.42
2:J:343:ARG:CZ	2:J:344:GLY:H	2.33	0.42
1:N:102:GLY:HA2	2:J:343:ARG:NH1	2.33	0.42
2:J:336:TRP:C	2:J:348:ILE:HD12	2.45	0.42
2:J:362:GLU:HB2	4:J:483:HOH:O	2.19	0.42
1:L:102:GLY:CA	2:H:343:ARG:HB3	2.49	0.42
2:J:359:LYS:HE3	4:J:482:HOH:O	2.20	0.42
2:H:383:LEU:HD12	4:H:91:HOH:O	2.20	0.42
2:J:376:SER:O	2:J:378:THR:HG23	2.20	0.42
1:N:69:ILE:HB	4:N:377:HOH:O	2.20	0.42
1:N:56:ARG:HD2	1:N:64:PHE:O	2.20	0.42
2:H:339:GLN:HA	2:H:344:GLY:O	2.20	0.42
1:N:98:TRP:N	4:N:385:HOH:O	2.40	0.42
1:N:93:TRP:NE1	1:N:95:SER:HA	2.35	0.41
2:I:402:TYR:CG	2:J:342:GLY:HA3	2.55	0.41
1:N:31:THR:C	1:N:33:ASN:H	2.28	0.41
2:J:381:MET:HE2	2:J:382:GLN:C	2.45	0.41
1:L:94:TYR:O	1:L:95:SER:C	2.63	0.41
2:I:379:ALA:HB1	4:I:458:HOH:O	2.20	0.41
2:J:318:VAL:HG22	2:J:386:LEU:HD21	2.01	0.41
2:H:343:ARG:HG3	4:H:108:HOH:O	2.20	0.41
2:H:350:ARG:HG3	3:H:430[B]:NPC:O3B	2.21	0.41
1:N:57:ALA:HA	2:J:406:TYR:CD2	2.55	0.41
2:J:336:TRP:CZ2	2:J:396:CYS:HB3	2.56	0.41
3:J:430:NPC:H72	3:J:430:NPC:H101	1.09	0.41
1:M:1:GLN:HG2	4:M:114:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:350:ARG:HD2	2:I:351:ILE:N	2.36	0.41
2:J:336:TRP:O	2:J:348:ILE:HD12	2.20	0.41
2:J:343:ARG:CD	2:J:344:GLY:H	2.34	0.41
2:I:343:ARG:HB2	4:I:462:HOH:O	2.20	0.41
2:J:323:LYS:HA	2:J:378:THR:CB	2.43	0.41
1:L:37:TRP:CZ3	1:L:90:CYS:HB3	2.56	0.40
2:H:318:VAL:HG13	4:H:91:HOH:O	2.21	0.40
2:I:350:ARG:HG3	3:I:430:NPC:O3B	2.21	0.40
1:N:16:GLU:HG3	4:N:337:HOH:O	2.21	0.40
2:J:351:ILE:CG1	2:J:372:VAL:HG13	2.51	0.40
2:J:353:PRO:O	2:J:374:LYS:HE3	2.21	0.40
2:J:374:LYS:CB	2:J:375:PRO:HD3	2.50	0.40
2:J:392:ALA:HA	4:J:469:HOH:O	2.20	0.40
2:H:389:GLU:HB2	2:H:390:ASP:OD1	2.21	0.40
1:N:92:LEU:HD21	4:N:379:HOH:O	2.21	0.40
2:J:335:HIS:CE1	2:J:347:TRP:HE1	2.38	0.40
2:J:347:TRP:HE3	2:J:361:ASN:ND2	2.19	0.40
2:J:374:LYS:N	2:J:375:PRO:CD	2.84	0.40
2:J:347:TRP:HB3	2:J:361:ASN:ND2	2.29	0.40
2:J:404:SER:O	2:J:405:SER:C	2.65	0.40
1:L:40:GLU:O	1:L:86:ALA:HB1	2.21	0.40
1:N:56:ARG:O	1:N:57:ALA:C	2.64	0.40
2:J:339:GLN:HB2	2:J:345:LEU:HD23	2.03	0.40
1:L:85:GLU:O	1:L:86:ALA:HB2	2.22	0.40
2:I:374:LYS:N	2:I:375:PRO:CD	2.85	0.40
1:N:60:VAL:HA	1:N:61:PRO:HD3	1.89	0.40
2:J:318:VAL:CG2	2:J:386:LEU:HD21	2.51	0.40
2:J:364:PHE:O	2:J:365:LYS:C	2.64	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	108/110 (98%)	95 (88%)	11 (10%)	2 (2%)	6	1
1	M	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	4	0
1	N	107/110 (97%)	87 (81%)	12 (11%)	8 (8%)	1	0
2	H	117/120 (98%)	99 (85%)	9 (8%)	9 (8%)	1	0
2	I	118/120 (98%)	111 (94%)	4 (3%)	3 (2%)	4	1
2	J	119/120 (99%)	89 (75%)	13 (11%)	17 (14%)	0	0
All	All	677/690 (98%)	575 (85%)	60 (9%)	42 (6%)	1	0

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	343	ARG
2	H	388	SER
2	H	390	ASP
1	M	62	ALA
2	I	343	ARG
2	I	366	SER
1	N	43	ASP
1	N	95	SER
2	J	317	SER
2	J	328	THR
2	J	329	PHE
2	J	356	GLY
2	J	371	THR
2	J	400	ASP
2	J	419	SER
2	H	384	SER
1	N	34	TYR
1	N	80	ALA
1	N	82	THR
2	J	331	SER
2	J	353	PRO
2	J	365	LYS
2	J	369	THR
2	J	405	SER
1	L	95	SER
2	H	329	PHE
2	H	341	PRO
2	H	391	SER
1	M	42	PRO
1	M	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	62	ALA
2	J	355	SER
2	J	385	SER
1	L	67	SER
2	H	386	LEU
2	I	404	SER
1	N	86	ALA
2	J	316	ALA
2	J	418	VAL
2	J	315	GLY
2	H	340	ARG
1	N	58	PRO

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	82/87 (94%)	73 (89%)	9 (11%)	6	1
1	M	87/87 (100%)	79 (91%)	8 (9%)	8	2
1	N	83/87 (95%)	66 (80%)	17 (20%)	1	0
2	H	101/102 (99%)	87 (86%)	14 (14%)	3	1
2	I	102/102 (100%)	85 (83%)	17 (17%)	2	0
2	J	99/102 (97%)	68 (69%)	31 (31%)	0	0
All	All	554/567 (98%)	458 (83%)	96 (17%)	2	0

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	11	THR
1	L	30	THR
1	L	31	THR
1	L	33	ASN
1	L	36	ASN
1	L	47	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	54	ASN
1	L	85	GLU
1	L	109	LEU
2	H	301	GLN
2	H	312	VAL
2	H	313	LYS
2	H	340	ARG
2	H	343	ARG
2	H	350	ARG
2	H	353	PRO
2	H	363	LYS
2	H	365	LYS
2	H	374	LYS
2	H	387	THR
2	H	406	TYR
2	H	412	GLN
2	H	417	THR
1	M	11	THR
1	M	41	LYS
1	M	42	PRO
1	M	45	LEU
1	M	68	LEU
1	M	75	LEU
1	M	96	ASN
1	M	109	LEU
2	I	303	GLN
2	I	305	GLN
2	I	311	LEU
2	I	319	LYS
2	I	320	LEU
2	I	321	SER
2	I	323	LYS
2	I	340	ARG
2	I	354	ASN
2	I	355	SER
2	I	359	LYS
2	I	362	GLU
2	I	367	LYS
2	I	374	LYS
2	I	389	GLU
2	I	406	TYR
2	I	417	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	8	SER
1	N	10	LEU
1	N	14	PRO
1	N	16	GLU
1	N	18	VAL
1	N	32	SER
1	N	33	ASN
1	N	43	ASP
1	N	45	LEU
1	N	56	ARG
1	N	68	LEU
1	N	75	LEU
1	N	78	THR
1	N	83	GLU
1	N	99	VAL
1	N	100	PHE
1	N	107	THR
2	J	304	LEU
2	J	312	VAL
2	J	318	VAL
2	J	320	LEU
2	J	323	LYS
2	J	331	SER
2	J	337	VAL
2	J	340	ARG
2	J	343	ARG
2	J	350	ARG
2	J	359	LYS
2	J	360	TYR
2	J	363	LYS
2	J	367[A]	LYS
2	J	367[B]	LYS
2	J	369	THR
2	J	370	LEU
2	J	372	VAL
2	J	373	ASP
2	J	374	LYS
2	J	376	SER
2	J	378	THR
2	J	381	MET
2	J	386	LEU
2	J	388	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	395	TYR
2	J	400	ASP
2	J	402	TYR
2	J	405	SER
2	J	406	TYR
2	J	417	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	36	ASN
1	L	55	ASN
1	L	96	ASN
2	H	335	HIS
2	H	354	ASN
2	H	412	GLN
1	M	81	GLN
1	M	96	ASN
1	M	97	HIS
2	I	301	GLN
2	I	303	GLN
2	I	335	HIS
2	I	354	ASN
1	N	33	ASN
1	N	36	ASN
1	N	55	ASN
2	J	303	GLN
2	J	354	ASN
2	J	361	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NPC	H	430[A]	-	22,22,22	1.90	6 (27%)	24,28,28	1.35	3 (12%)
3	NPC	I	430	-	22,22,22	2.08	8 (36%)	24,28,28	2.38	6 (25%)
3	NPC	J	430	-	22,22,22	1.60	5 (22%)	24,28,28	3.09	9 (37%)
3	NPC	H	430[B]	-	22,22,22	2.81	8 (36%)	24,28,28	1.64	5 (20%)

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	NPC	H	430[A]	-	-	7/15/17/17	0/1/1/1
3	NPC	I	430	-	-	4/15/17/17	0/1/1/1
3	NPC	J	430	-	-	9/15/17/17	0/1/1/1
3	NPC	H	430[B]	-	-	7/15/17/17	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	430[B]	NPC	C2-C3	7.53	1.53	1.39
3	H	430[B]	NPC	C5-C4	6.75	1.51	1.39
3	H	430[B]	NPC	C2-C1	4.75	1.47	1.39
3	I	430	NPC	C14-C15	4.49	1.61	1.50
3	H	430[A]	NPC	C14-C15	-4.44	1.40	1.50
3	J	430	NPC	C7-C1	-4.05	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	430[A]	NPC	C7-C1	-4.01	1.45	1.51
3	I	430	NPC	C7-C1	-3.99	1.45	1.51
3	H	430[B]	NPC	C6-C5	3.62	1.44	1.38
3	I	430	NPC	O16-C15	-3.22	1.20	1.30
3	I	430	NPC	C10-N9	-3.07	1.39	1.46
3	H	430[A]	NPC	O4-C4	3.02	1.42	1.36
3	J	430	NPC	O4-C4	3.02	1.42	1.36
3	I	430	NPC	O15-C15	-2.97	1.12	1.22
3	H	430[A]	NPC	C3-N3	-2.81	1.40	1.45
3	I	430	NPC	O4-C4	2.81	1.42	1.36
3	H	430[B]	NPC	C14-C15	2.81	1.57	1.50
3	J	430	NPC	C10-N9	-2.71	1.40	1.46
3	H	430[B]	NPC	C10-N9	-2.57	1.40	1.46
3	I	430	NPC	C12-C11	2.52	1.64	1.51
3	H	430[A]	NPC	C10-N9	-2.35	1.40	1.46
3	H	430[B]	NPC	C12-C11	2.23	1.62	1.51
3	J	430	NPC	C12-C11	2.16	1.62	1.51
3	H	430[A]	NPC	C12-C11	2.15	1.62	1.51
3	I	430	NPC	C7-C8	-2.14	1.47	1.52
3	J	430	NPC	O15-C15	-2.05	1.15	1.22
3	H	430[B]	NPC	O15-C15	-2.05	1.15	1.22

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	430	NPC	O8-C8-C7	8.37	140.13	121.99
3	I	430	NPC	O16-C15-O15	6.80	140.81	123.33
3	J	430	NPC	C7-C8-N9	-6.17	107.50	116.06
3	J	430	NPC	C10-N9-C8	-5.97	111.70	122.82
3	J	430	NPC	O8-C8-N9	-5.43	112.37	123.03
3	I	430	NPC	O16-C15-C14	-4.73	99.07	114.00
3	I	430	NPC	C7-C8-N9	4.18	121.85	116.06
3	I	430	NPC	C13-C14-C15	-3.70	104.86	114.51
3	J	430	NPC	C11-C10-N9	3.42	121.79	112.20
3	J	430	NPC	C13-C14-C15	3.39	123.35	114.51
3	H	430[B]	NPC	C13-C14-C15	-3.33	105.82	114.51
3	H	430[B]	NPC	C6-C5-C4	3.30	123.80	120.50
3	H	430[B]	NPC	C2-C3-C4	-3.18	117.35	121.42
3	H	430[A]	NPC	C13-C14-C15	3.05	122.46	114.51
3	J	430	NPC	O4-C4-C5	-2.95	111.44	119.36
3	J	430	NPC	O4-C4-C3	2.90	129.97	121.32
3	I	430	NPC	C2-C3-C4	-2.86	117.76	121.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	430[B]	NPC	C7-C8-N9	2.72	119.84	116.06
3	H	430[A]	NPC	O16-C15-O15	-2.72	116.34	123.33
3	J	430	NPC	O3B-N3-C3	-2.51	114.73	119.03
3	H	430[A]	NPC	C1-C7-C8	2.37	119.41	112.33
3	I	430	NPC	O8-C8-N9	-2.22	118.68	123.03
3	H	430[B]	NPC	C3-C2-C1	2.04	122.82	118.55

There are no chirality outliers.

All (27) torsion outliers are listed below:

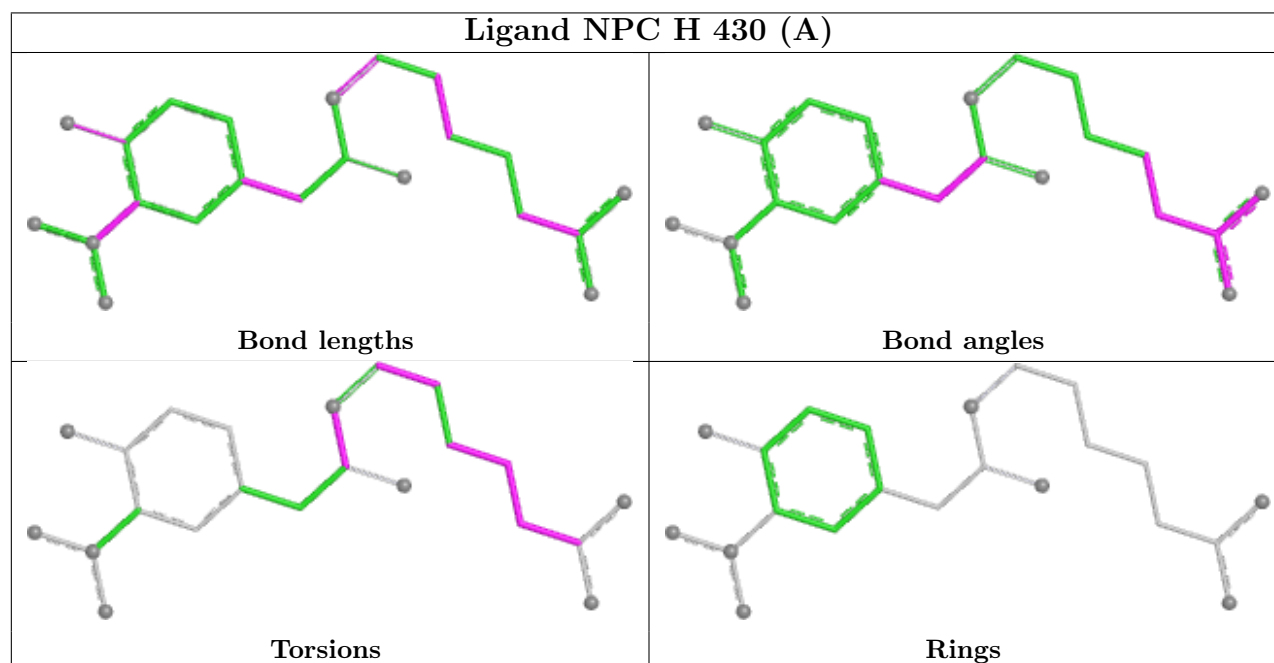
Mol	Chain	Res	Type	Atoms
3	H	430[A]	NPC	C7-C8-N9-C10
3	I	430	NPC	C7-C8-N9-C10
3	I	430	NPC	O8-C8-N9-C10
3	H	430[A]	NPC	O8-C8-N9-C10
3	J	430	NPC	C7-C8-N9-C10
3	H	430[B]	NPC	O8-C8-N9-C10
3	J	430	NPC	N9-C10-C11-C12
3	J	430	NPC	O8-C8-N9-C10
3	H	430[A]	NPC	C12-C13-C14-C15
3	H	430[A]	NPC	N9-C10-C11-C12
3	H	430[B]	NPC	N9-C10-C11-C12
3	H	430[B]	NPC	C7-C8-N9-C10
3	H	430[B]	NPC	C11-C12-C13-C14
3	H	430[A]	NPC	C11-C12-C13-C14
3	J	430	NPC	C6-C1-C7-C8
3	H	430[B]	NPC	C10-C11-C12-C13
3	J	430	NPC	C2-C1-C7-C8
3	I	430	NPC	C10-C11-C12-C13
3	J	430	NPC	C10-C11-C12-C13
3	I	430	NPC	N9-C10-C11-C12
3	J	430	NPC	C11-C12-C13-C14
3	H	430[B]	NPC	C1-C7-C8-N9
3	J	430	NPC	C13-C14-C15-O15
3	J	430	NPC	C13-C14-C15-O16
3	H	430[B]	NPC	C1-C7-C8-O8
3	H	430[A]	NPC	C13-C14-C15-O16
3	H	430[A]	NPC	C13-C14-C15-O15

There are no ring outliers.

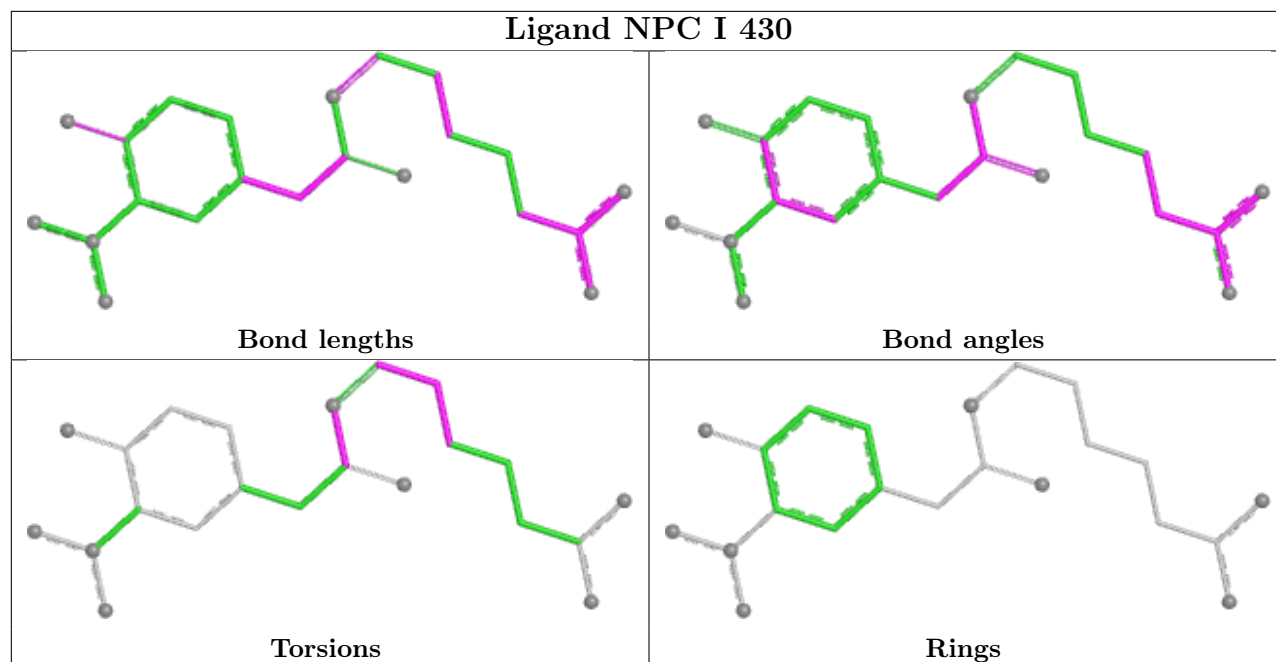
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	430[A]	NPC	2	0
3	I	430	NPC	3	0
3	J	430	NPC	1	0
3	H	430[B]	NPC	1	0

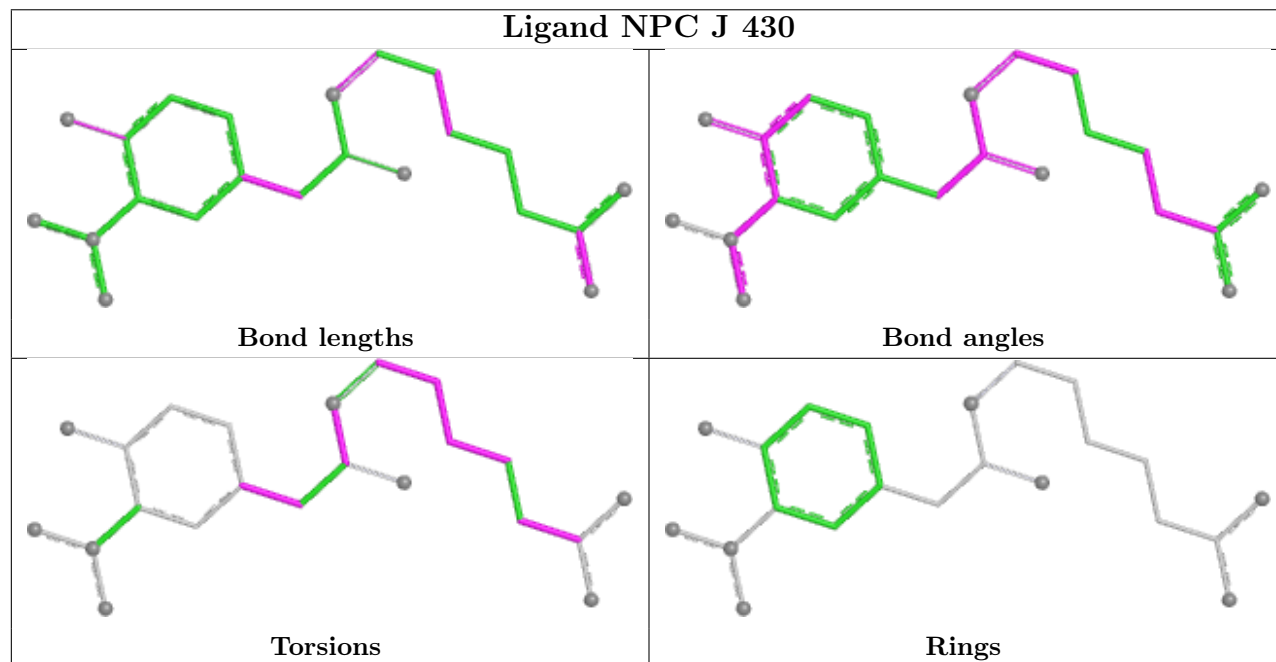
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

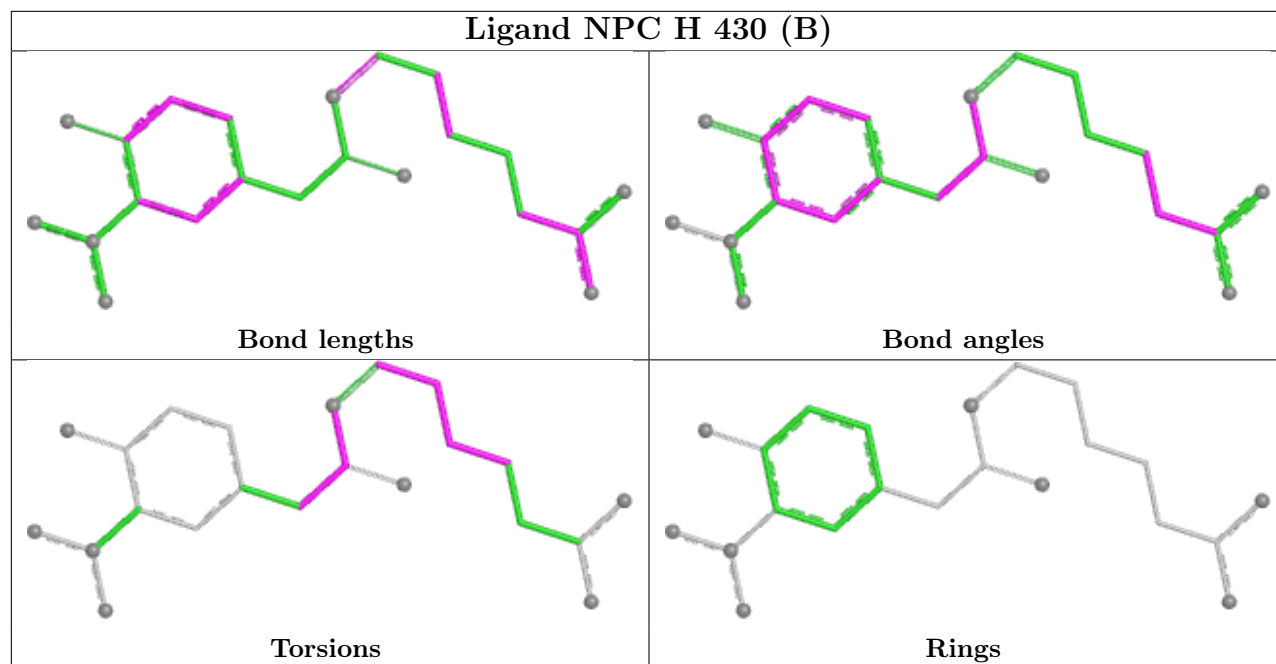


Ligand NPC I 430



Ligand NPC J 430





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.