Full wwPDB X-ray Structure Validation Report (i)

Jun 7, 2023 – 02:01 PM EDT

PDB ID	:	1A6V
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 (i) 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 (1)) were used in the production of this report:

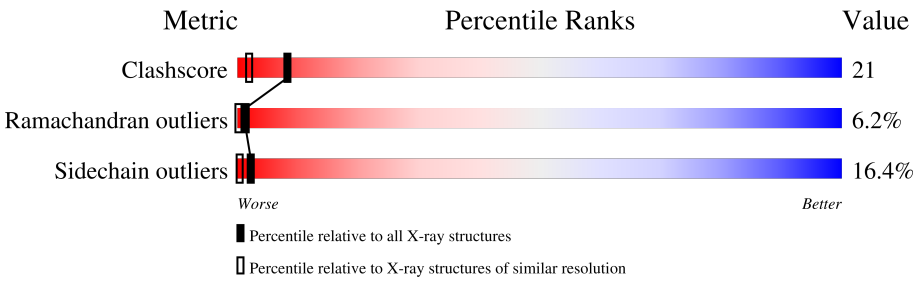
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	110	64% 34% •
1	M	110	63% 28% 6% • •
1	N	110	37% 43% 16% • •
2	H	120	48% 37% 10% • •
2	I	120	52% 37% 8% • •
2	J	120	28% 38% 28% 7%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	L	110	799	503	134	160	2	0	0	0
1	M	109	814	513	139	160	2	0	1	0
1	N	109	799	503	136	158	2	0	0	0

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).

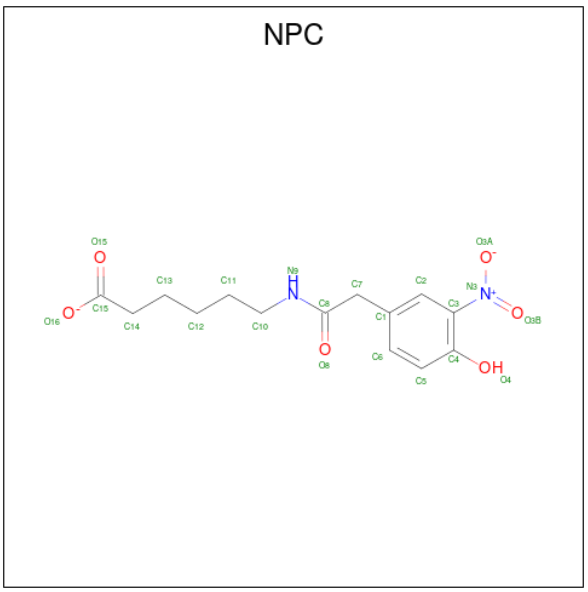
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	118	936	597	154	181	4	0	1	0
2	I	119	942	600	155	183	4	0	1	0
2	J	120	942	601	156	181	4	0	1	0

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 (three-letter code: 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		

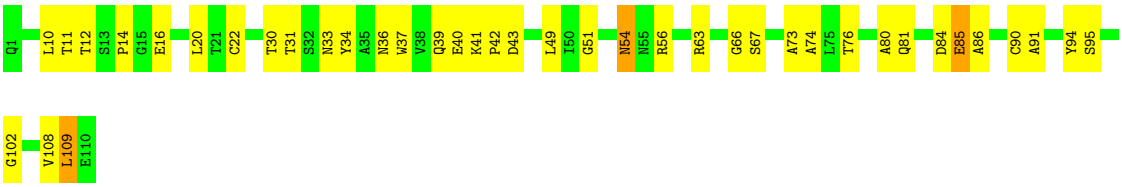
3 Residue-property plots (i)

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.

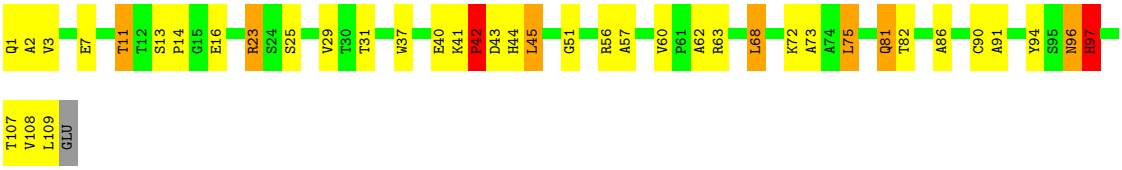
• Molecule 1: B1-8 FV (LIGHT CHAIN)

Chain L:



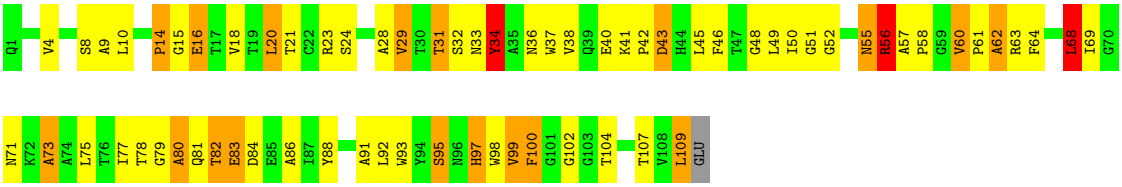
• Molecule 1: B1-8 FV (LIGHT CHAIN)

Chain M:



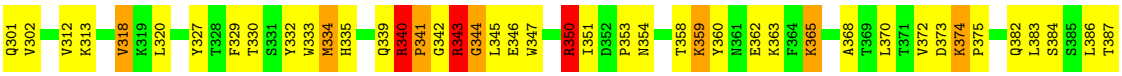
• Molecule 1: B1-8 FV (LIGHT CHAIN)

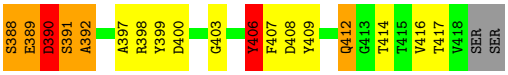
Chain N:



• Molecule 2: B1-8 FV (HEAVY CHAIN)

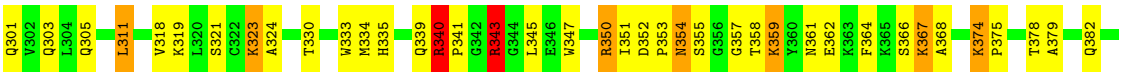
Chain H:





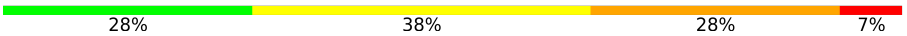
• Molecule 2: B1-8 FV (HEAVY CHAIN)

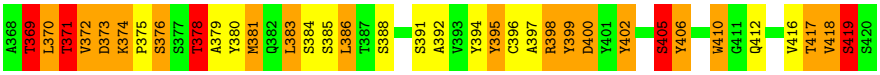
Chain I:



• Molecule 2: B1-8 FV (HEAVY CHAIN)

Chain J:





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	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 (i)

5.1 Standard geometry (i)

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	0.89	0/817	1.83	13/1119 (1.2%)
1	M	0.90	1/837 (0.1%)	1.93	23/1144 (2.0%)
1	N	0.91	1/816 (0.1%)	2.18	35/1115 (3.1%)
2	H	0.88	0/968	2.06	38/1313 (2.9%)
2	I	0.84	0/974	1.78	15/1321 (1.1%)
2	J	0.88	0/974	2.31	38/1320 (2.9%)
All	All	0.88	2/5386 (0.0%)	2.03	162/7332 (2.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	82	THR	C-O	6.44	1.35	1.23
1	M	7	GLU	CD-OE1	-5.35	1.19	1.25

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	398	ARG	NE-CZ-NH1	23.59	132.09	120.30
1	N	63	ARG	CD-NE-CZ	18.49	149.49	123.60
2	H	343	ARG	NE-CZ-NH2	-15.39	112.61	120.30
2	J	398	ARG	NE-CZ-NH2	-15.17	112.71	120.30
1	L	63	ARG	NE-CZ-NH2	-13.57	113.51	120.30
1	N	63	ARG	NE-CZ-NH2	13.42	127.01	120.30
1	N	23	ARG	NE-CZ-NH1	13.34	126.97	120.30
2	J	418	VAL	C-N-CA	12.46	152.84	121.70
1	M	56	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	M	63	ARG	NE-CZ-NH1	11.95	126.27	120.30
2	H	389	GLU	C-N-CA	11.85	151.32	121.70
1	N	63	ARG	NE-CZ-NH1	-11.16	114.72	120.30
2	J	398	ARG	CD-NE-CZ	11.09	139.13	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	359	LYS	CA-CB-CG	10.64	136.81	113.40
2	H	403	GLY	N-CA-C	10.42	139.14	113.10
2	I	408	ASP	CB-CG-OD1	10.35	127.61	118.30
2	J	340	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	M	56	ARG	CD-NE-CZ	9.45	136.83	123.60
2	H	350	ARG	NE-CZ-NH1	9.36	124.98	120.30
2	J	340	ARG	CD-NE-CZ	9.23	136.52	123.60
2	J	346	GLU	CA-CB-CG	9.22	133.68	113.40
1	L	63	ARG	NE-CZ-NH1	9.13	124.86	120.30
2	J	399	TYR	CB-CG-CD1	9.02	126.41	121.00
1	N	34	TYR	CB-CG-CD2	8.45	126.07	121.00
2	I	340	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	N	23	ARG	CD-NE-CZ	8.33	135.26	123.60
2	H	343	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	I	350	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	H	350	ARG	CA-CB-CG	8.10	131.22	113.40
2	H	343	ARG	N-CA-CB	7.83	124.69	110.60
2	J	322	CYS	CA-CB-SG	7.82	128.08	114.00
1	M	56	ARG	CA-CB-CG	7.78	130.52	113.40
1	M	43	ASP	CB-CG-OD1	7.78	125.30	118.30
2	J	369	THR	N-CA-CB	7.73	124.98	110.30
2	J	320	LEU	CA-CB-CG	7.71	133.02	115.30
1	M	45	LEU	CB-CA-C	7.70	124.83	110.20
2	I	389	GLU	CA-CB-CG	7.60	130.13	113.40
2	J	373	ASP	CB-CG-OD1	7.54	125.08	118.30
2	H	334	MET	CG-SD-CE	7.45	112.12	100.20
2	J	410	TRP	CA-CB-CG	7.42	127.80	113.70
1	N	55	ASN	CB-CA-C	7.27	124.94	110.40
1	M	16	GLU	CA-CB-CG	7.19	129.22	113.40
2	J	399	TYR	CB-CG-CD2	-7.18	116.69	121.00
2	J	355	SER	C-N-CA	7.12	137.25	122.30
2	I	340	ARG	NE-CZ-NH1	7.10	123.85	120.30
2	J	394	TYR	CB-CG-CD2	-7.04	116.77	121.00
2	J	343	ARG	NE-CZ-NH2	7.01	123.80	120.30
2	H	408	ASP	CB-CG-OD1	7.00	124.59	118.30
2	H	390	ASP	CB-CG-OD2	6.94	124.54	118.30
2	J	371	THR	N-CA-CB	6.84	123.30	110.30
2	H	373	ASP	CB-CG-OD1	6.82	124.44	118.30
1	N	34	TYR	CG-CD2-CE2	6.80	126.74	121.30
1	L	91	ALA	N-CA-CB	6.78	119.59	110.10
1	M	23	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	H	343	ARG	CA-CB-CG	6.74	128.22	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	91	ALA	N-CA-CB	-6.74	100.67	110.10
1	N	34	TYR	CG-CD1-CE1	6.72	126.68	121.30
1	N	20	LEU	CB-CA-C	6.69	122.91	110.20
2	J	352	ASP	N-CA-CB	6.67	122.61	110.60
2	H	389	GLU	CA-C-O	6.66	134.09	120.10
1	N	84	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	J	378	THR	CA-CB-CG2	6.63	121.68	112.40
2	H	388	SER	N-CA-CB	6.62	120.43	110.50
2	I	415	THR	CA-CB-CG2	6.60	121.64	112.40
2	J	373	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	H	318	VAL	CA-CB-CG1	6.58	120.77	110.90
2	H	342	GLY	C-N-CA	6.56	138.11	121.70
1	M	16	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	N	4	VAL	CA-CB-CG1	6.40	120.50	110.90
2	J	366	SER	N-CA-CB	-6.39	100.91	110.50
1	L	42	PRO	C-N-CA	6.39	137.66	121.70
2	I	395	TYR	CB-CG-CD1	-6.38	117.17	121.00
2	J	395	TYR	CA-CB-CG	6.33	125.42	113.40
1	N	18	VAL	N-CA-CB	6.32	125.40	111.50
1	N	34	TYR	CD1-CG-CD2	-6.27	111.00	117.90
2	H	406	TYR	CA-CB-CG	6.27	125.31	113.40
2	J	340	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	M	2	ALA	N-CA-C	-6.26	94.09	111.00
2	H	346	GLU	N-CA-CB	6.26	121.86	110.60
2	H	350	ARG	CG-CD-NE	6.18	124.77	111.80
1	M	23	ARG	CA-CB-CG	6.17	126.97	113.40
1	N	81	GLN	C-N-CA	6.15	137.08	121.70
1	M	81	GLN	CB-CG-CD	6.12	127.52	111.60
2	J	327	TYR	CA-CB-CG	6.12	125.03	113.40
1	N	56	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	N	29	VAL	CA-CB-CG2	6.11	120.07	110.90
2	H	340	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	N	84	ASP	CB-CG-OD1	6.08	123.77	118.30
1	N	99	VAL	CB-CA-C	6.03	122.86	111.40
1	L	76	THR	CA-CB-OG1	-6.00	96.41	109.00
1	N	40	GLU	CG-CD-OE1	5.89	130.09	118.30
1	M	81	GLN	CA-CB-CG	5.87	126.32	113.40
2	J	333	TRP	CB-CA-C	5.85	122.10	110.40
2	H	344	GLY	CA-C-O	-5.84	110.08	120.60
2	H	362	GLU	CG-CD-OE1	5.84	129.99	118.30
1	N	83	GLU	CG-CD-OE1	5.83	129.96	118.30
2	H	373	ASP	CB-CG-OD2	-5.81	113.07	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	345	LEU	CA-C-O	5.81	132.30	120.10
2	H	399	TYR	CB-CG-CD2	5.79	124.48	121.00
1	N	21	THR	C-N-CA	5.76	136.10	121.70
2	H	409	TYR	CB-CG-CD2	5.74	124.44	121.00
1	L	94	TYR	N-CA-CB	5.73	120.91	110.60
2	J	355	SER	N-CA-C	5.71	126.41	111.00
2	J	405	SER	N-CA-CB	-5.71	101.94	110.50
2	I	343	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	J	320	LEU	CB-CA-C	5.66	120.95	110.20
1	N	82	THR	CA-C-O	-5.64	108.26	120.10
1	M	31	THR	CA-CB-CG2	5.63	120.28	112.40
1	N	109	LEU	CB-CA-C	5.62	120.88	110.20
2	I	324	ALA	N-CA-CB	-5.61	102.24	110.10
2	J	345	LEU	N-CA-C	5.58	126.07	111.00
2	H	392	ALA	N-CA-CB	-5.57	102.30	110.10
2	H	340	ARG	N-CA-CB	5.56	120.61	110.60
1	N	23	ARG	NH1-CZ-NH2	-5.55	113.29	119.40
1	M	23	ARG	NH1-CZ-NH2	-5.53	113.31	119.40
2	H	344	GLY	N-CA-C	5.53	126.91	113.10
1	M	16	GLU	CG-CD-OE1	5.42	129.15	118.30
1	N	68	LEU	CA-CB-CG	5.42	127.78	115.30
2	J	394	TYR	CB-CG-CD1	5.42	124.25	121.00
1	M	90	CYS	N-CA-CB	5.41	120.34	110.60
1	M	23	ARG	NE-CZ-NH2	5.41	123.00	120.30
2	H	372	VAL	CA-CB-CG2	5.41	119.01	110.90
1	N	29	VAL	N-CA-CB	5.38	123.34	111.50
2	H	345	LEU	CA-CB-CG	5.37	127.66	115.30
1	L	43	ASP	C-N-CA	5.37	135.12	121.70
1	L	43	ASP	CB-CA-C	5.37	121.13	110.40
2	J	343	ARG	CD-NE-CZ	5.36	131.11	123.60
2	H	350	ARG	CD-NE-CZ	5.36	131.10	123.60
2	H	333	TRP	CB-CA-C	5.35	121.11	110.40
2	H	399	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	N	73	ALA	N-CA-CB	5.34	117.58	110.10
1	L	54	ASN	CA-CB-CG	5.33	125.12	113.40
1	N	18	VAL	CA-CB-CG2	5.32	118.89	110.90
1	L	84	ASP	CB-CG-OD1	5.30	123.07	118.30
2	I	358	THR	CA-CB-CG2	5.30	119.81	112.40
2	J	340	ARG	N-CA-CB	5.28	120.11	110.60
1	L	34	TYR	CB-CA-C	5.28	120.95	110.40
1	M	97	HIS	CA-CB-CG	5.24	122.50	113.60
1	M	68	LEU	CA-CB-CG	5.20	127.25	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	359	LYS	N-CA-CB	5.16	119.89	110.60
2	J	402	TYR	N-CA-CB	5.16	119.89	110.60
1	N	88	TYR	CB-CG-CD2	-5.16	117.91	121.00
2	H	390	ASP	OD1-CG-OD2	-5.14	113.53	123.30
2	I	396	CYS	N-CA-C	-5.14	97.12	111.00
2	H	332	TYR	CB-CG-CD2	-5.14	117.92	121.00
2	J	310	GLU	CG-CD-OE1	5.12	128.55	118.30
1	N	34	TYR	CA-CB-CG	5.12	123.14	113.40
2	J	383	LEU	O-C-N	5.12	130.89	122.70
1	N	107	THR	CA-CB-CG2	5.12	119.56	112.40
2	J	417	THR	CB-CA-C	5.11	125.39	111.60
2	I	406	TYR	CA-CB-CG	5.09	123.07	113.40
2	I	390	ASP	N-CA-CB	5.06	119.71	110.60
2	H	350	ARG	CB-CG-CD	5.05	124.74	111.60
1	M	63	ARG	CD-NE-CZ	5.05	130.66	123.60
2	I	367	LYS	CA-CB-CG	5.04	124.49	113.40
1	N	60	VAL	CA-CB-CG1	5.04	118.45	110.90
1	N	31	THR	CB-CA-C	5.03	125.18	111.60
1	M	56	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
2	I	408	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	L	16	GLU	CA-CB-CG	5.02	124.44	113.40
1	N	29	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	L	56	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	799	0	756	19	0
1	M	814	0	796	18	0
1	N	799	0	769	44	0
2	H	936	0	893	40	0
2	I	942	0	899	38	0
2	J	942	0	891	73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	44	0	34	5	0
3	I	22	0	17	3	0
3	J	22	0	17	1	0
4	H	81	0	0	8	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
4	N	68	0	0	9	0
All	All	5798	0	5072	219	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 21.

All (219) 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)
3:H:430[A]:NPC:H112	4:H:73:HOH:O	1.47	1.12
3:H:430[B]:NPC:O8	4:H:73:HOH:O	1.71	1.06
1:N:56:ARG:NH2	4:N:365:HOH:O	1.86	0.85
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
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:HE21	2:H:412:GLN:H	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: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:H101	3:I:430:NPC:H6	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:J:304:LEU:HD22	2:J:334:MET:HE1	1.86	0.58
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:312:VAL:C	2:J:419:SER:HB3	2.27	0.54
2:H:330:THR:HB	2:H:354:ASN:ND2	2.23	0.54
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
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:H:350:ARG:HH21	2:H:359:LYS:CD	2.25	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
2:J:304:LEU:HB3	2:J:334:MET:HE1	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:350:ARG:HD2	2:H:350:ARG:C	2.34	0.47
1:L:22:CYS:HB3	1:L:73:ALA:HB3	1.96	0.47
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
1:L:12:THR:HG23	1:L:108:VAL:HA	1.97	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:J:341:PRO:C	2:J:343:ARG:H	2.17	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
1:M:81:GLN:C	1:M:108:VAL:HG11	2.36	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:334:MET:HE3	2:H:397:ALA:N	2.33	0.43
1:M:40:GLU:O	1:M:86:ALA:HB1	2.18	0.43
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
1:N:109:LEU:C	1:N:109:LEU:HD13	2.39	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
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: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:M:13:SER:O	1:M:14:PRO:C	2.57	0.41
1:N:51:GLY:O	1:N:52:GLY:C	2.58	0.41
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:381:MET:HE2	2:J:383:LEU:N	2.36	0.40
2:J:392:ALA:HA	4:J:469:HOH:O	2.20	0.40
1:L:81:GLN:C	1:L:108:VAL:HG21	2.40	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
1:L:40:GLU:O	1:L:86:ALA:HB1	2.21	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

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%)	8	1
1	M	108/110 (98%)	94 (87%)	11 (10%)	3 (3%)	5	1
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%)	5	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	391	SER
1	M	42	PRO
1	M	96	ASN
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	82/87 (94%)	74 (90%)	8 (10%)	8 2
1	M	87/87 (100%)	78 (90%)	9 (10%)	7 2
1	N	83/87 (95%)	68 (82%)	15 (18%)	1 0
2	H	101/102 (99%)	88 (87%)	13 (13%)	4 1
2	I	102/102 (100%)	86 (84%)	16 (16%)	2 0
2	J	99/102 (97%)	69 (70%)	30 (30%)	0 0
All	All	554/567 (98%)	463 (84%)	91 (16%)	2 0

All (91) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	33	ASN
1	L	36	ASN
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	363	LYS
2	H	365	LYS
2	H	374	LYS
2	H	387	THR
2	H	400	ASP
2	H	406	TYR
2	H	412	GLN
1	M	11	THR
1	M	42	PRO
1	M	44	HIS
1	M	45	LEU
1	M	68	LEU
1	M	75	LEU
1	M	96	ASN
1	M	97	HIS
1	M	109	LEU
2	I	303	GLN
2	I	305	GLN
2	I	311	LEU
2	I	319	LYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	417	THR
1	N	8	SER
1	N	10	LEU
1	N	14	PRO
1	N	16	GLU
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	97	HIS
1	N	100	PHE
2	J	301	GLN
2	J	304	LEU
2	J	312	VAL
2	J	318	VAL
2	J	320	LEU
2	J	331	SER
2	J	340	ARG
2	J	343	ARG
2	J	350	ARG
2	J	359	LYS
2	J	360	TYR
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
2	J	395	TYR
2	J	400	ASP
2	J	402	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	405	SER
2	J	406	TYR
2	J	417	THR
2	J	419	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	96	ASN
2	H	335	HIS
2	H	354	ASN
2	H	412	GLN
1	M	1	GLN
1	M	55	ASN
1	M	96	ASN
1	M	97	HIS
2	I	301	GLN
2	I	335	HIS
2	I	354	ASN
2	I	412	GLN
1	N	33	ASN
1	N	36	ASN
2	J	303	GLN
2	J	354	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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[B]	-	21,22,22	2.82	8 (38%)	24,28,28	1.62	5 (20%)
3	NPC	H	430[A]	-	21,22,22	1.89	5 (23%)	24,28,28	1.37	3 (12%)
3	NPC	J	430	-	21,22,22	1.57	4 (19%)	24,28,28	3.09	9 (37%)
3	NPC	I	430	-	21,22,22	2.06	7 (33%)	24,28,28	2.40	6 (25%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	430[B]	NPC	C2-C3	7.67	1.53	1.39
3	H	430[B]	NPC	C5-C4	6.58	1.51	1.39
3	H	430[B]	NPC	C2-C1	4.71	1.47	1.39
3	I	430	NPC	C14-C15	4.47	1.61	1.50
3	H	430[A]	NPC	C14-C15	-4.42	1.40	1.50
3	J	430	NPC	C7-C1	-4.00	1.45	1.51
3	H	430[A]	NPC	C7-C1	-3.96	1.45	1.51
3	I	430	NPC	C7-C1	-3.95	1.45	1.51
3	H	430[B]	NPC	C6-C5	3.25	1.44	1.38
3	I	430	NPC	O16-C15	-3.14	1.20	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	430	NPC	C10-N9	-3.01	1.39	1.46
3	H	430[A]	NPC	O4-C4	2.96	1.42	1.36
3	J	430	NPC	O4-C4	2.95	1.42	1.36
3	I	430	NPC	O15-C15	-2.95	1.12	1.22
3	H	430[A]	NPC	C3-N3	-2.81	1.40	1.45
3	H	430[B]	NPC	C14-C15	2.79	1.57	1.50
3	I	430	NPC	O4-C4	2.75	1.42	1.36
3	J	430	NPC	C10-N9	-2.66	1.40	1.46
3	H	430[B]	NPC	C10-N9	-2.52	1.40	1.46
3	H	430[A]	NPC	C10-N9	-2.31	1.40	1.46
3	I	430	NPC	C12-C11	2.27	1.64	1.51
3	J	430	NPC	O15-C15	-2.04	1.15	1.22
3	H	430[B]	NPC	O15-C15	-2.04	1.15	1.22
3	H	430[B]	NPC	C12-C11	2.01	1.62	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	430	NPC	O8-C8-C7	7.95	140.13	122.03
3	I	430	NPC	O16-C15-O15	7.03	140.81	123.30
3	J	430	NPC	C7-C8-N9	-6.43	107.50	116.19
3	J	430	NPC	C10-N9-C8	-6.00	111.70	122.84
3	J	430	NPC	O8-C8-N9	-5.64	112.37	123.01
3	I	430	NPC	O16-C15-C14	-4.66	99.07	114.03
3	I	430	NPC	C7-C8-N9	4.19	121.85	116.19
3	I	430	NPC	C13-C14-C15	-3.81	104.86	114.47
3	J	430	NPC	C13-C14-C15	3.52	123.35	114.47
3	H	430[B]	NPC	C13-C14-C15	-3.43	105.82	114.47
3	J	430	NPC	C11-C10-N9	3.35	121.79	112.21
3	H	430[B]	NPC	C6-C5-C4	3.21	123.80	120.50
3	H	430[A]	NPC	C13-C14-C15	3.17	122.46	114.47
3	H	430[B]	NPC	C2-C3-C4	-3.10	117.35	121.45
3	J	430	NPC	O4-C4-C3	2.93	129.97	121.31
3	J	430	NPC	O4-C4-C5	-2.90	111.44	119.33
3	I	430	NPC	C2-C3-C4	-2.79	117.76	121.45
3	H	430[A]	NPC	O16-C15-O15	-2.79	116.34	123.30
3	H	430[B]	NPC	C7-C8-N9	2.70	119.84	116.19
3	J	430	NPC	O3B-N3-C3	-2.51	114.73	119.03
3	H	430[A]	NPC	C1-C7-C8	2.31	119.41	112.57
3	I	430	NPC	O8-C8-N9	-2.29	118.68	123.01
3	H	430[B]	NPC	C3-C2-C1	2.01	122.82	118.54

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	J	430	NPC	C2-C1-C7-C8
3	H	430[B]	NPC	C10-C11-C12-C13
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.

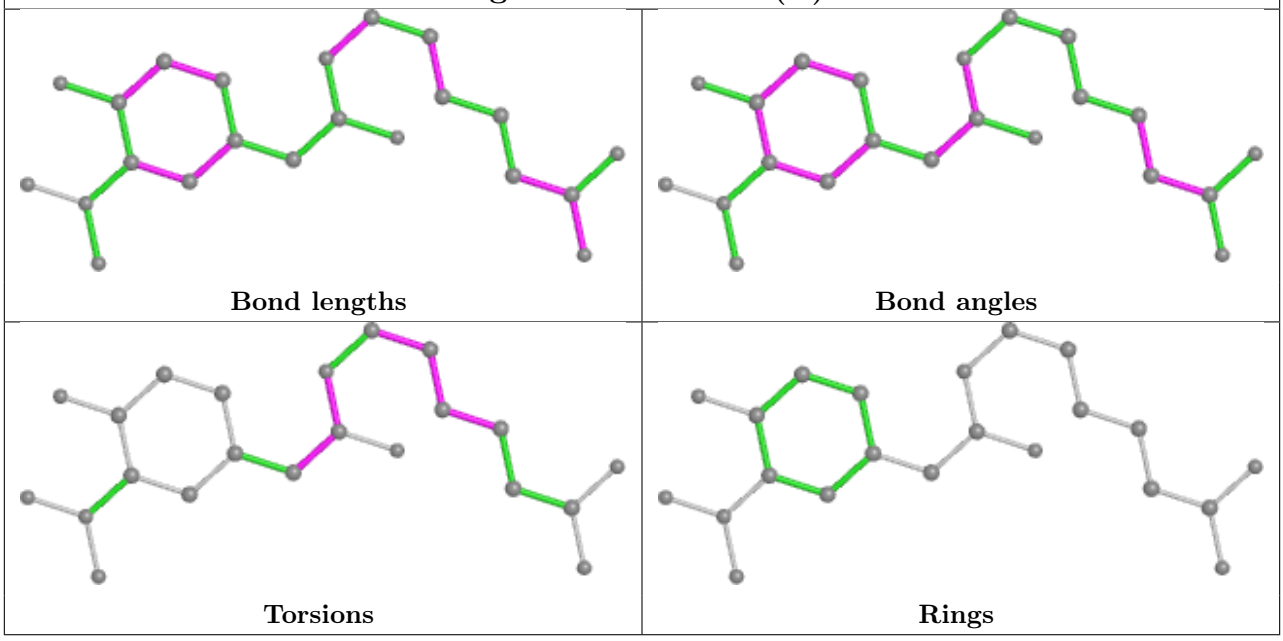
4 monomers are involved in 9 short contacts:

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

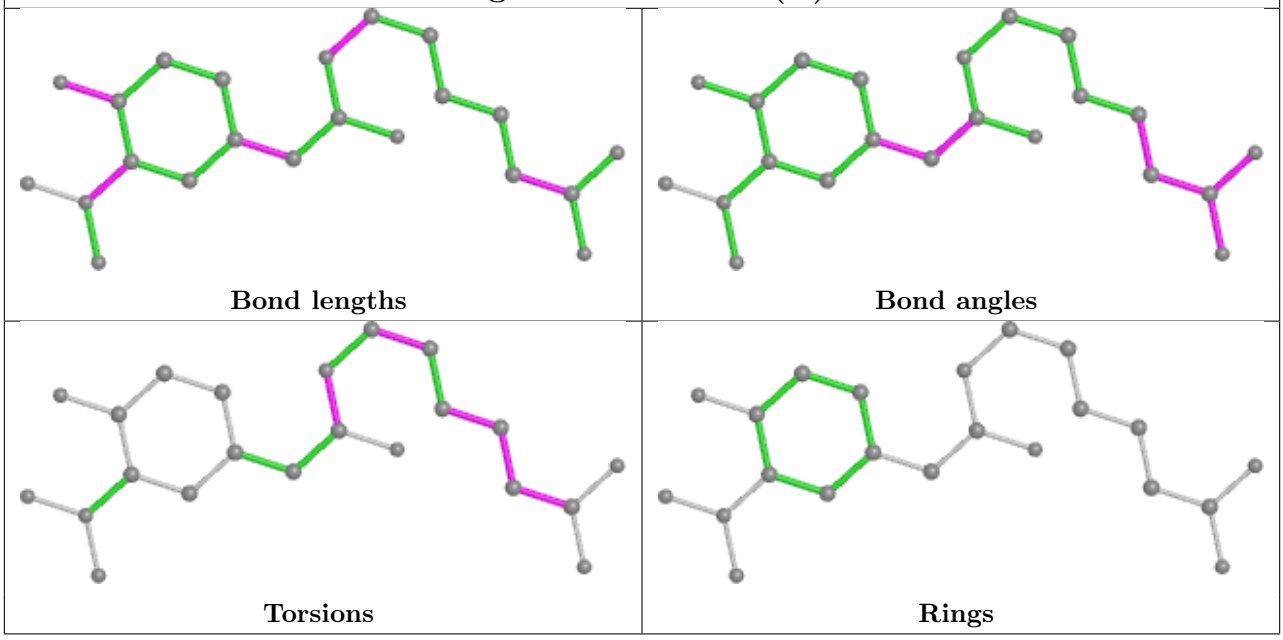
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

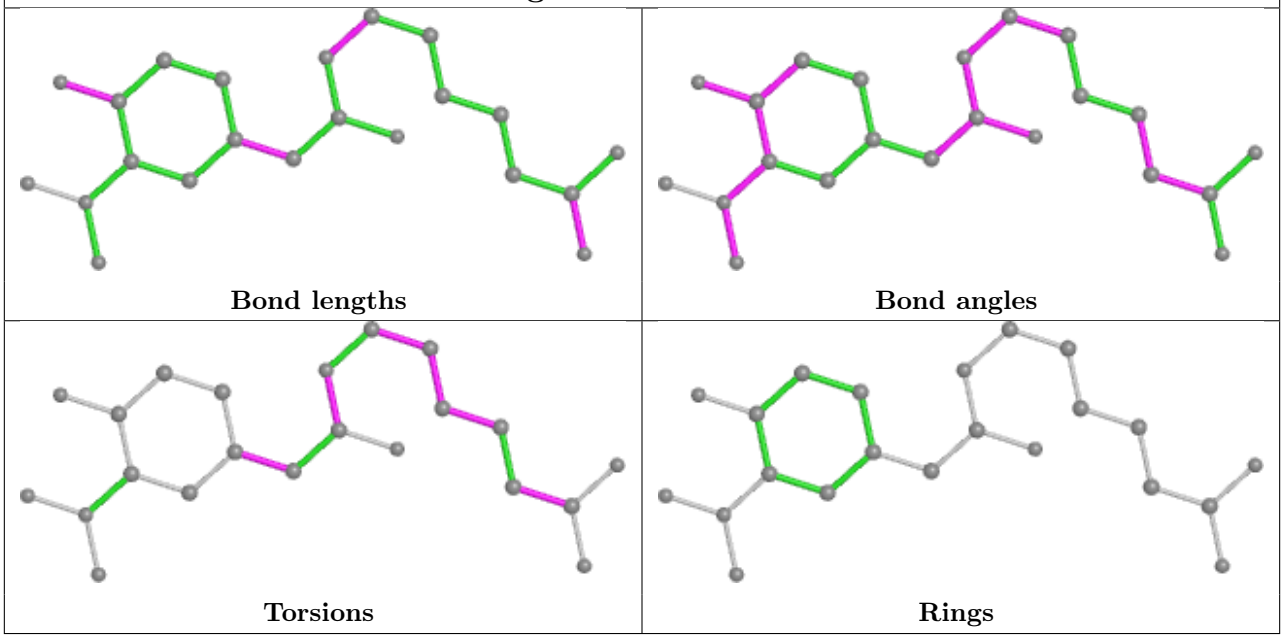
Ligand NPC H 430 (B)



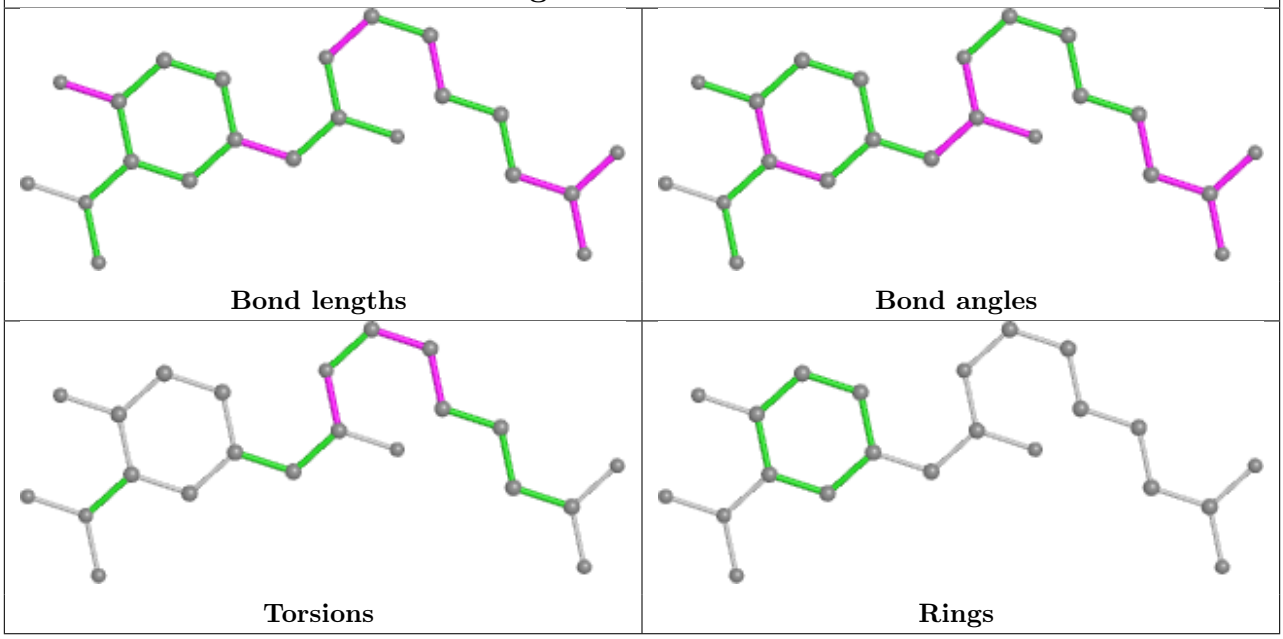
Ligand NPC H 430 (A)



Ligand NPC J 430



Ligand NPC I 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.