



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:28 PM UTC

PDB ID : 1BAF / pdb_00001baf
Title : 2.9 ANGSTROMS RESOLUTION STRUCTURE OF AN ANTI-DINITRO
PHENYL-SPIN-LABEL MONOCLONAL ANTIBODY FAB FRAGMENT
WITH BOUND HAPTEN
Authors : Leahy, D.J.; Brunger, A.T.; Fox, R.O.; Hynes, T.R.
Deposited on : 1992-01-16
Resolution : 2.90 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

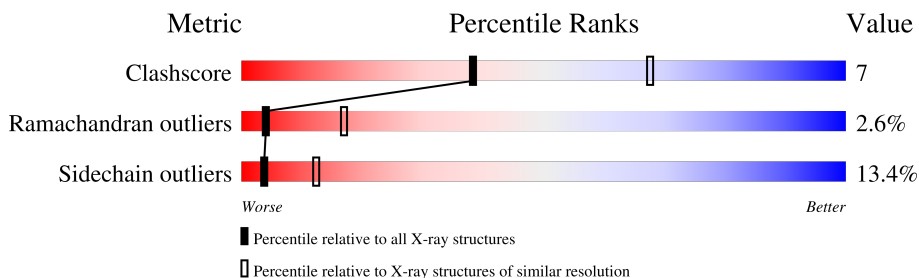
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	214	 56% 36% 7% •
2	H	217	 64% 26% 8% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4082 atoms, of which 740 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IGG1-KAPPA AN02 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	214	Total	C	H	N	O	S	0	0	0
			2031	1033	378	272	338	10			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	17	GLU	GLN	conflict	GB 437099
L	21	MET	ILE	conflict	GB 437099
L	?	-	SER	deletion	GB 437099
L	?	-	SER	deletion	GB 437099
L	30	TYR	ARG	conflict	GB 437099
L	31	TYR	PHE	conflict	GB 437099
L	32	MET	LEU	conflict	GB 437099
L	33	TYR	HIS	conflict	GB 437099
L	39	PRO	SER	conflict	GB 437099
L	41	SER	ALA	conflict	GB 437099
L	44	ARG	LYS	conflict	GB 437099
L	46	LEU	TRP	conflict	GB 437099
L	52	ASN	LYS	conflict	GB 437099
L	55	SER	PRO	conflict	GB 437099
L	59	VAL	ALA	conflict	GB 437099
L	76	ARG	SER	conflict	GB 437099
L	84	THR	SER	conflict	GB 437099
L	86	TYR	PHE	conflict	GB 437099
L	88	GLN	HIS	conflict	GB 437099
L	94	PRO	-	insertion	GB 437099
L	96	ILE	LEU	conflict	GB 437099
L	100	VAL	ALA	conflict	GB 437099

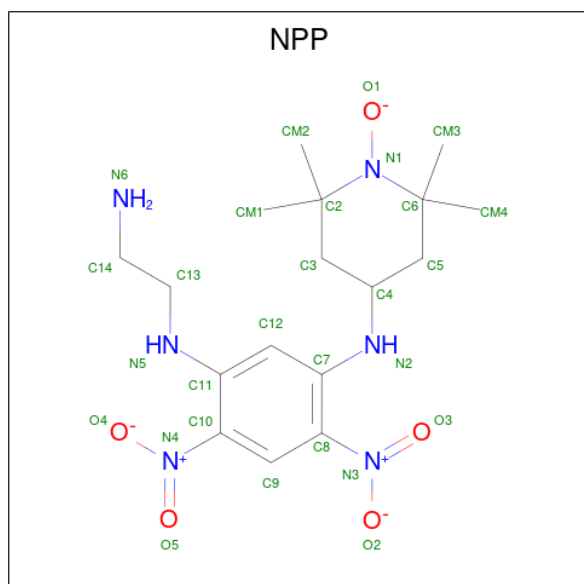
- Molecule 2 is a protein called IGG1-KAPPA AN02 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	217	Total	C	H	N	O	S	0	0	0
			2023	1048	362	278	327	8			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	18	GLN	LEU	conflict	GB 1513182
H	29	ILE	VAL	conflict	GB 1513182
H	32	ASP	GLU	conflict	GB 1513182
H	49	MET	LEU	conflict	GB 1513182
H	52	MET	ILE	conflict	GB 1513182
H	53	SER	ASN	conflict	GB 1513182
H	59	ARG	SER	conflict	GB 1513182
H	65	ARG	LYS	conflict	GB 1513182
H	84	LYS	ASN	conflict	GB 1513182
H	95	PHE	TYR	conflict	GB 1513182
H	?	-	ASP	deletion	GB 1513182
H	99	GLY	SER	conflict	GB 1513182
H	101	PRO	-	insertion	GB 1513182
H	102	LEU	PHE	conflict	GB 1513182
H	110	GLN	LEU	conflict	GB 1513182
H	112	SER	THR	conflict	GB 1513182
H	115	GLU	ALA	conflict	GB 1513182
H	189	PRO	THR	conflict	GB 1513182
H	190	ARG	TRP	conflict	GB 1513182

- Molecule 3 is N-(2-AMINO-ETHYL)-4,6-DINITRO-N'-(2,2,6,6-TETRAMETHYL-1-OXY-PIPERIDIN-4-YL)-BENZENE-1,3-DIAMINE (CCD ID: NPP) (formula: $C_{17}H_{27}N_6O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	1	Total	C	N	O	0	0
			28	17	6	5		

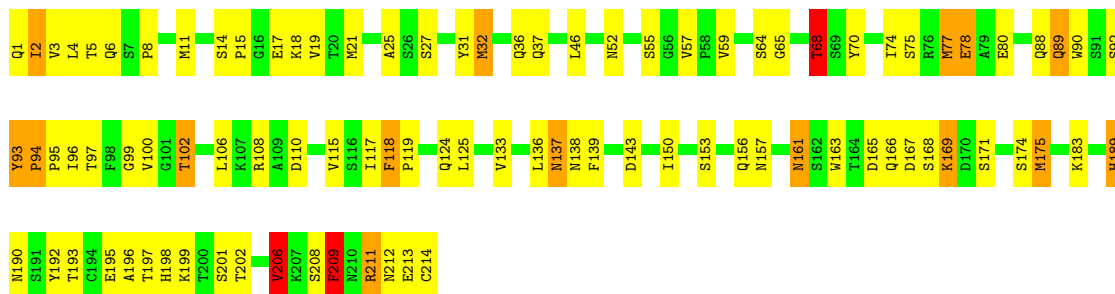
3 Residue-property plots [i](#)

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.

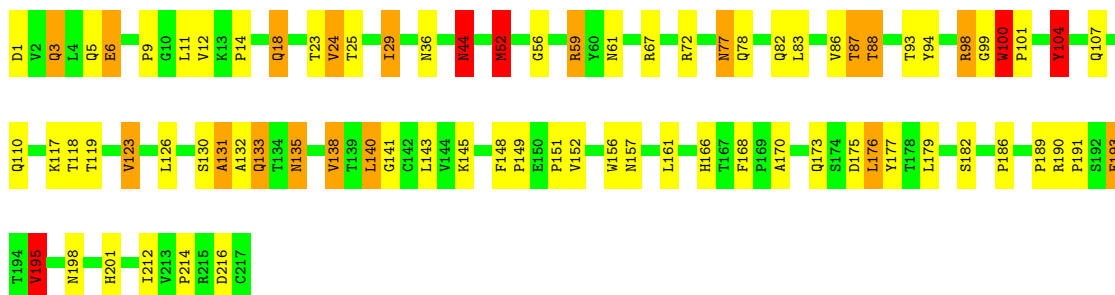
- Molecule 1: IGG1-KAPPA AN02 FAB (LIGHT CHAIN)

Chain L: 



- Molecule 2: IGG1-KAPPA AN02 FAB (HEAVY CHAIN)

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	73.23Å 73.23Å 373.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4082	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: NPP

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	1.02	4/1693 (0.2%)	2.04	56/2303 (2.4%)
2	H	1.05	5/1707 (0.3%)	2.07	55/2337 (2.4%)
All	All	1.04	9/3400 (0.3%)	2.06	111/4640 (2.4%)

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
2	H	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	201	HIS	CD2-NE2	-7.06	1.30	1.37
1	L	198	HIS	CD2-NE2	-7.02	1.30	1.37
2	H	24	VAL	CA-CB	6.92	1.63	1.54
1	L	206	VAL	CA-CB	6.63	1.61	1.53
2	H	166	HIS	CD2-NE2	-6.07	1.31	1.37
2	H	123	VAL	CA-CB	6.05	1.61	1.54
1	L	150	ILE	CA-CB	6.05	1.60	1.53
1	L	189	HIS	CD2-NE2	-5.96	1.31	1.37
2	H	83	LEU	CA-CB	-5.65	1.45	1.53

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	138	ASN	OD1-CG-ND2	-12.04	110.56	122.60
1	L	137	ASN	OD1-CG-ND2	-10.91	111.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	18	GLN	OE1-CD-NE2	-10.91	111.69	122.60
2	H	173	GLN	OE1-CD-NE2	-10.88	111.72	122.60
2	H	135	ASN	OD1-CG-ND2	-10.86	111.74	122.60
1	L	190	ASN	OD1-CG-ND2	-9.60	113.00	122.60
2	H	216	ASP	CA-CB-CG	9.42	122.02	112.60
1	L	156	GLN	OE1-CD-NE2	-9.29	113.31	122.60
1	L	94	PRO	N-CA-C	8.99	121.66	110.70
1	L	32	MET	CA-CB-CG	-8.67	96.76	114.10
2	H	198	ASN	OD1-CG-ND2	-8.64	113.96	122.60
2	H	135	ASN	CA-CB-CG	8.52	121.12	112.60
1	L	36	GLN	OE1-CD-NE2	-8.23	114.37	122.60
2	H	157	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	L	157	ASN	OD1-CG-ND2	-8.19	114.41	122.60
1	L	57	VAL	N-CA-C	7.95	116.79	107.73
1	L	68	THR	CA-CB-OG1	-7.78	97.93	109.60
2	H	44	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	L	110	ASP	CA-CB-CG	7.50	120.11	112.60
1	L	55	SER	N-CA-C	7.50	119.24	111.14
1	L	161	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	L	6	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	L	190	ASN	CB-CG-ND2	7.24	127.25	116.40
2	H	110	GLN	OE1-CD-NE2	-7.20	115.40	122.60
2	H	135	ASN	N-CA-C	7.20	117.38	107.73
2	H	61	ASN	OD1-CG-ND2	-7.10	115.50	122.60
2	H	133	GLN	OE1-CD-NE2	-7.07	115.53	122.60
2	H	86	VAL	N-CA-C	7.04	118.87	109.37
2	H	138	VAL	CB-CA-C	-7.02	101.30	110.84
1	L	212	ASN	OD1-CG-ND2	-6.89	115.71	122.60
1	L	2	ILE	N-CA-C	6.82	123.52	109.34
2	H	99	GLY	N-CA-C	6.76	123.58	111.62
1	L	3	VAL	N-CA-C	6.75	117.80	108.89
1	L	137	ASN	N-CA-C	6.62	120.82	110.17
1	L	37	GLN	OE1-CD-NE2	-6.61	115.99	122.60
2	H	107	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	L	209	PHE	CA-CB-CG	6.52	120.32	113.80
2	H	135	ASN	CB-CG-ND2	6.50	126.15	116.40
1	L	89	GLN	N-CA-C	6.50	120.28	109.95
1	L	78	GLU	O-C-N	-6.49	115.67	122.94
1	L	99	GLY	O-C-N	-6.46	117.67	122.71
1	L	166	GLN	OE1-CD-NE2	-6.44	116.16	122.60
2	H	3	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	L	139	PHE	N-CA-C	6.38	119.92	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	131	ALA	N-CA-C	6.26	124.13	110.80
1	L	52	ASN	OD1-CG-ND2	-6.25	116.35	122.60
2	H	78	GLN	OE1-CD-NE2	-6.25	116.35	122.60
2	H	141	GLY	N-CA-C	6.24	119.60	110.80
2	H	61	ASN	CA-C-N	6.21	126.67	119.47
2	H	61	ASN	C-N-CA	6.21	126.67	119.47
2	H	88	THR	CA-CB-OG1	-6.19	100.31	109.60
1	L	90	TRP	CE2-CD2-CE3	6.18	124.98	118.80
1	L	68	THR	CA-CB-CG2	6.16	120.97	110.50
2	H	18	GLN	CG-CD-NE2	6.16	125.64	116.40
2	H	216	ASP	N-CA-CB	-6.15	100.10	110.49
2	H	36	ASN	N-CA-C	6.11	119.56	110.52
1	L	137	ASN	CB-CG-ND2	6.10	125.55	116.40
1	L	6	GLN	N-CA-C	6.07	119.94	110.17
2	H	24	VAL	CA-C-O	6.04	127.61	120.72
1	L	133	VAL	N-CA-C	6.03	117.70	108.71
2	H	82	GLN	OE1-CD-NE2	-6.01	116.59	122.60
2	H	52	MET	CA-CB-CG	-6.01	102.08	114.10
1	L	17	GLU	N-CA-C	5.99	118.94	110.50
1	L	156	GLN	O-C-N	-5.95	115.79	122.34
2	H	77	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	L	165	ASP	CA-CB-CG	-5.89	106.71	112.60
2	H	138	VAL	N-CA-CB	5.88	118.04	110.99
1	L	88	GLN	OE1-CD-NE2	-5.81	116.79	122.60
2	H	198	ASN	CB-CG-ND2	5.81	125.11	116.40
1	L	96	ILE	N-CA-CB	5.75	117.38	110.31
2	H	100	TRP	CG-CD2-CE3	5.72	139.62	133.90
2	H	152	VAL	CB-CA-C	-5.67	103.08	111.19
1	L	1	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	H	195	VAL	O-C-N	-5.65	117.38	123.14
1	L	118	PHE	CA-C-N	5.62	126.17	120.38
1	L	118	PHE	C-N-CA	5.62	126.17	120.38
2	H	177	TYR	N-CA-C	5.59	118.80	110.52
2	H	145	LYS	CB-CG-CD	-5.59	98.45	111.30
1	L	138	ASN	CB-CG-ND2	5.58	124.78	116.40
1	L	36	GLN	CG-CD-NE2	5.54	124.71	116.40
1	L	157	ASN	CA-CB-CG	5.53	118.13	112.60
2	H	67	ARG	N-CA-C	5.53	118.50	111.69
2	H	173	GLN	CG-CD-NE2	5.52	124.69	116.40
1	L	1	GLN	CG-CD-NE2	5.52	124.68	116.40
2	H	100	TRP	CB-CG-CD1	-5.50	118.65	126.90
2	H	193	GLU	CA-C-O	5.48	126.62	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	L	124	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	L	138	ASN	N-CA-C	5.46	118.78	111.24
1	L	93	TYR	N-CA-C	5.36	121.64	109.81
2	H	212	ILE	O-C-N	-5.33	116.17	122.77
2	H	24	VAL	N-CA-C	5.32	116.24	108.53
1	L	208	SER	N-CA-C	5.32	117.06	108.34
2	H	88	THR	CA-CB-CG2	5.24	119.40	110.50
1	L	117	ILE	CA-C-O	5.20	126.49	120.67
1	L	167	ASP	N-CA-C	5.20	117.76	110.23
2	H	123	VAL	CA-C-O	5.15	125.75	120.39
2	H	72	ARG	N-CA-C	5.14	116.88	109.07
2	H	100	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	H	170	ALA	N-CA-C	5.10	117.29	110.35
1	L	143	ASP	CA-CB-CG	-5.09	107.51	112.60
2	H	52	MET	CG-SD-CE	-5.09	89.70	100.90
1	L	206	VAL	N-CA-C	5.08	115.08	107.51
1	L	89	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	H	176	LEU	O-C-N	-5.04	117.63	123.33
1	L	161	ASN	CB-CG-ND2	5.03	123.94	116.40
2	H	87	THR	O-C-N	-5.02	117.31	122.94
1	L	157	ASN	O-C-N	-5.02	117.13	122.85
2	H	175	ASP	CA-CB-CG	-5.02	107.58	112.60
1	L	211	ARG	N-CA-C	5.02	121.48	110.80
2	H	156	TRP	CE2-CD2-CG	-5.01	101.19	107.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	104	TYR	Sidechain

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	1653	378	1582	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1661	362	1617	19	0
3	L	28	0	27	2	0
All	All	3342	740	3226	45	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 7.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:GLN:HB3	2:H:25:THR:HB	1.56	0.87
2:H:190:ARG:HD2	2:H:191:PRO:HA	1.78	0.64
1:L:25:ALA:HB3	1:L:68:THR:HA	1.80	0.63
1:L:65:GLY:HA3	1:L:70:TYR:CD2	2.34	0.63
2:H:186:PRO:HB2	2:H:189:PRO:HD2	1.81	0.62
2:H:98:ARG:HB2	2:H:104:TYR:HB2	1.80	0.62
1:L:137:ASN:HD22	1:L:174:SER:HB3	1.66	0.61
1:L:8:PRO:HD2	1:L:11:MET:HE2	1.82	0.58
1:L:8:PRO:O	1:L:102:THR:HB	2.04	0.56
2:H:9:PRO:HG2	2:H:18:GLN:NE2	2.20	0.56
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.06	0.56
1:L:19:VAL:HB	1:L:74:ILE:HB	1.87	0.56
1:L:32:MET:HE2	1:L:89:GLN:HB3	1.88	0.54
1:L:77:MET:HE2	1:L:78:GLU:O	2.08	0.54
1:L:115:VAL:HG22	1:L:136:LEU:HD12	1.92	0.51
2:H:117:LYS:O	2:H:119:THR:HG23	2.11	0.50
1:L:119:PRO:HB3	1:L:209:PHE:CZ	2.46	0.50
1:L:163:TRP:NE1	1:L:175:MET:HE3	2.27	0.49
1:L:2:ILE:HG22	1:L:94:PRO:HB2	1.92	0.49
1:L:168:SER:OG	1:L:169:LYS:HG2	2.12	0.48
1:L:70:TYR:CD1	1:L:70:TYR:N	2.81	0.48
2:H:6:GLU:HG3	2:H:94:TYR:O	2.14	0.48
1:L:93:TYR:CE2	2:H:59:ARG:HG2	2.48	0.48
2:H:140:LEU:HD13	2:H:195:VAL:HG21	1.95	0.47
1:L:89:GLN:NE2	1:L:97:THR:H	2.13	0.47
1:L:15:PRO:HD3	1:L:106:LEU:HD22	1.98	0.46
1:L:136:LEU:HD11	1:L:196:ALA:HB2	1.99	0.45
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.78	0.45
1:L:118:PHE:CD2	2:H:126:LEU:HB3	2.52	0.45
2:H:191:PRO:HG3	2:H:214:PRO:HG3	1.99	0.45
2:H:9:PRO:HG2	2:H:18:GLN:CD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:TRP:HA	2:H:101:PRO:HA	1.87	0.44
1:L:100:VAL:O	2:H:44:ASN:ND2	2.50	0.44
1:L:31:TYR:CE2	3:L:250:NPP:HM41	2.53	0.43
2:H:29:ILE:HG12	2:H:77:ASN:OD1	2.18	0.43
2:H:190:ARG:HA	2:H:191:PRO:HA	1.72	0.43
1:L:11:MET:HE1	1:L:21:MET:HE2	1.99	0.43
1:L:137:ASN:HD21	2:H:168:PHE:HZ	1.66	0.42
1:L:108:ARG:HD2	1:L:171:SER:HB2	2.01	0.42
1:L:161:ASN:HB3	1:L:175:MET:HE2	2.01	0.42
1:L:195:GLU:HG3	1:L:206:VAL:HB	2.02	0.42
2:H:52:MET:HE3	2:H:56:GLY:HA2	2.02	0.42
1:L:18:LYS:HA	1:L:75:SER:O	2.20	0.41
3:L:250:NPP:H12	3:L:250:NPP:H4	1.93	0.40
2:H:148:PHE:HA	2:H:149:PRO:HA	1.82	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	212/214 (99%)	193 (91%)	16 (8%)	3 (1%)	9	30
2	H	215/217 (99%)	189 (88%)	18 (8%)	8 (4%)	2	11
All	All	427/431 (99%)	382 (90%)	34 (8%)	11 (3%)	4	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	44	ASN
2	H	118	THR
2	H	131	ALA
1	L	211	ARG

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Mol	Chain	Res	Type
1	L	201	SER
2	H	130	SER
2	H	132	ALA
2	H	29	ILE
2	H	104	TYR
2	H	100	TRP
1	L	59	VAL

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	190/190 (100%)	165 (87%)	25 (13%)	4	13
2	H	192/192 (100%)	166 (86%)	26 (14%)	4	12
All	All	382/382 (100%)	331 (87%)	51 (13%)	4	12

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	LEU
1	L	5	THR
1	L	14	SER
1	L	27	SER
1	L	46	LEU
1	L	64	SER
1	L	68	THR
1	L	77	MET
1	L	80	GLU
1	L	92	SER
1	L	95	PRO
1	L	102	THR
1	L	125	LEU
1	L	153	SER
1	L	169	LYS
1	L	175	MET

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Mol	Chain	Res	Type
1	L	183	LYS
1	L	193	THR
1	L	197	THR
1	L	199	LYS
1	L	202	THR
1	L	206	VAL
1	L	209	PHE
1	L	213	GLU
1	L	214	CYS
2	H	1	ASP
2	H	6	GLU
2	H	11	LEU
2	H	12	VAL
2	H	14	PRO
2	H	23	THR
2	H	24	VAL
2	H	52	MET
2	H	59	ARG
2	H	87	THR
2	H	88	THR
2	H	93	THR
2	H	98	ARG
2	H	123	VAL
2	H	133	GLN
2	H	135	ASN
2	H	138	VAL
2	H	140	LEU
2	H	143	LEU
2	H	151	PRO
2	H	161	LEU
2	H	176	LEU
2	H	179	LEU
2	H	182	SER
2	H	193	GLU
2	H	195	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	137	ASN
1	L	189	HIS

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Mol	Chain	Res	Type
1	L	210	ASN
2	H	40	GLN
2	H	78	GLN
2	H	133	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NPP	L	250	-	29,29,29	2.14	8 (27%)	36,44,44	1.46	7 (19%)

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	NPP	L	250	-	-	1/12/38/38	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	250	NPP	C7-N2	5.35	1.49	1.37
3	L	250	NPP	C11-N5	4.60	1.49	1.37
3	L	250	NPP	C2-N1	3.63	1.53	1.48
3	L	250	NPP	O1-N1	-3.43	1.25	1.43
3	L	250	NPP	C6-N1	3.36	1.53	1.48
3	L	250	NPP	C13-N5	2.68	1.51	1.45
3	L	250	NPP	C9-C8	-2.57	1.34	1.39
3	L	250	NPP	C9-C10	-2.48	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	250	NPP	C8-C7-N2	-3.65	119.75	123.45
3	L	250	NPP	C5-C6-N1	3.27	112.80	108.66
3	L	250	NPP	CM3-C6-C5	-2.81	103.66	110.22
3	L	250	NPP	C12-C7-C8	2.62	119.83	116.66
3	L	250	NPP	C3-C2-N1	2.23	111.48	108.66
3	L	250	NPP	C12-C11-C10	2.06	119.14	116.66
3	L	250	NPP	C7-N2-C4	-2.00	121.32	124.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	250	NPP	N5-C13-C14-N6

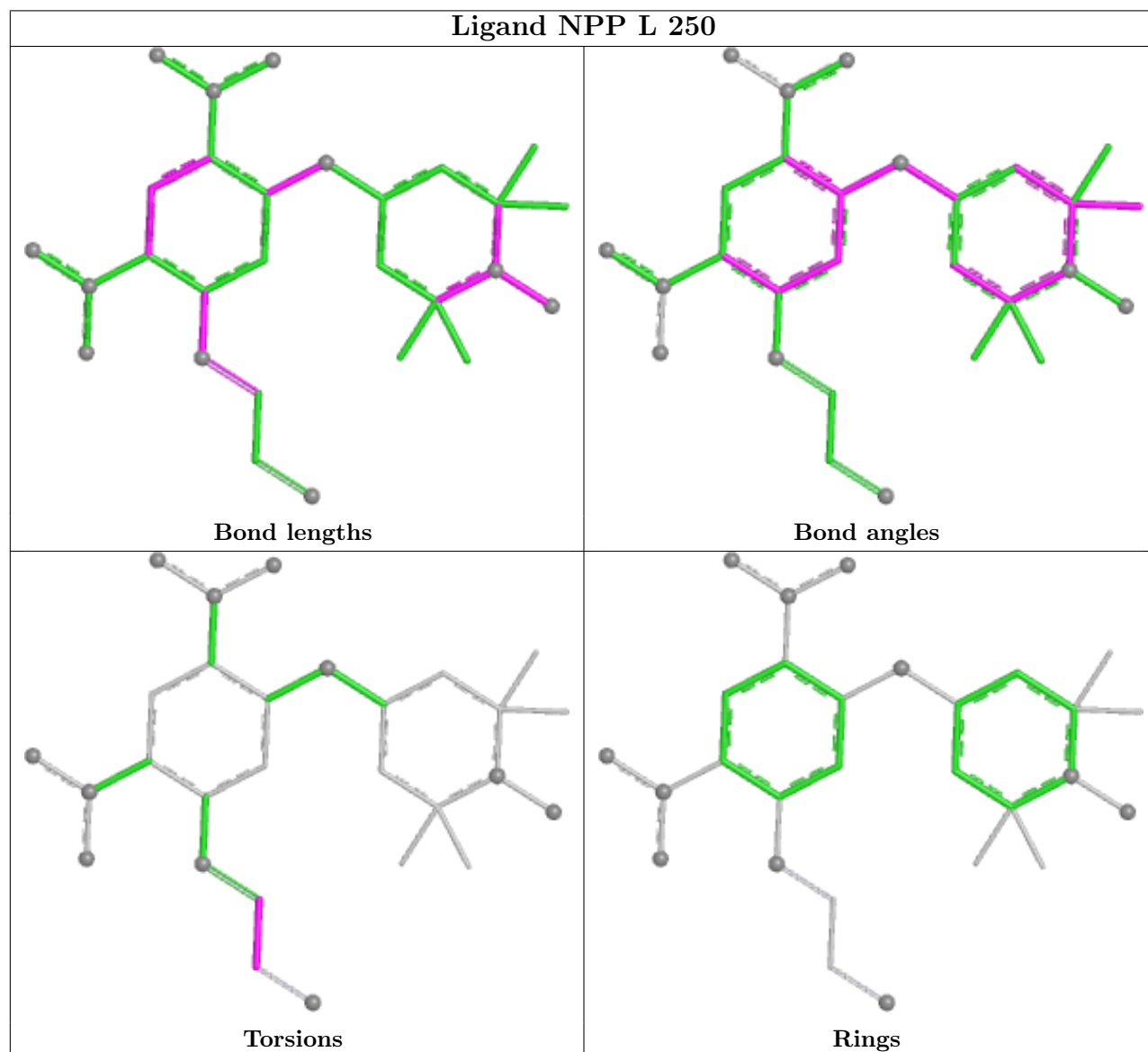
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	250	NPP	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 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.



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.