



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:24 PM UTC

PDB ID : 3GZN / pdb_00003gzn
Title : Structure of NEDD8-activating enzyme in complex with NEDD8 and MLN4924
Authors : Sintchak, M.D.
Deposited on : 2009-04-07
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

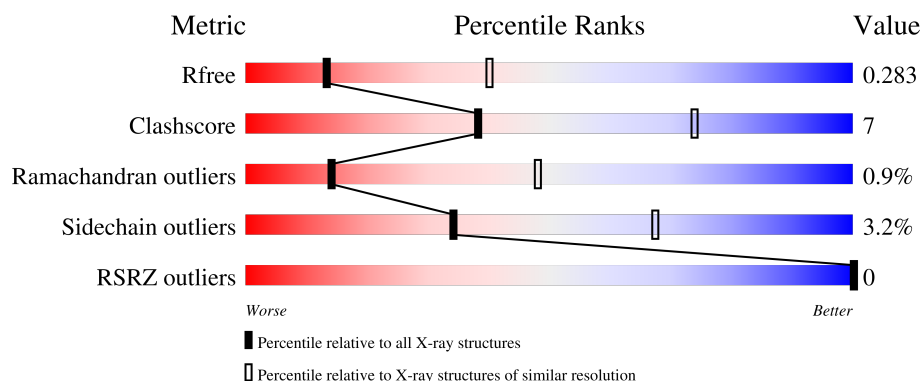
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

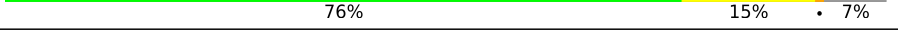
The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	 82% 16% ..
1	C	534	 84% 13% ..
2	B	463	 75% 16% • 7%
2	D	463	 76% 15% • 7%
3	I	82	 77% 20% •

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Mol	Chain	Length	Quality of chain
3	J	82	 78%18%.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16050 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 NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4095	2587	695	797	16			
1	C	526	Total	C	N	O	S	0	0	0
			4065	2573	687	789	16			

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3311	2119	558	616	18			
2	D	429	Total	C	N	O	S	0	0	0
			3320	2127	558	617	18			

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	79	Total	C	N	O	S	0	0	0
			593	373	102	116	2			
3	J	79	Total	C	N	O	S	0	0	0
			602	380	103	117	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-5	HIS	-	expression tag	UNP Q15843
I	-4	HIS	-	expression tag	UNP Q15843
I	-3	HIS	-	expression tag	UNP Q15843
I	-2	HIS	-	expression tag	UNP Q15843
I	-1	HIS	-	expression tag	UNP Q15843
I	0	HIS	-	expression tag	UNP Q15843
J	-5	HIS	-	expression tag	UNP Q15843
J	-4	HIS	-	expression tag	UNP Q15843

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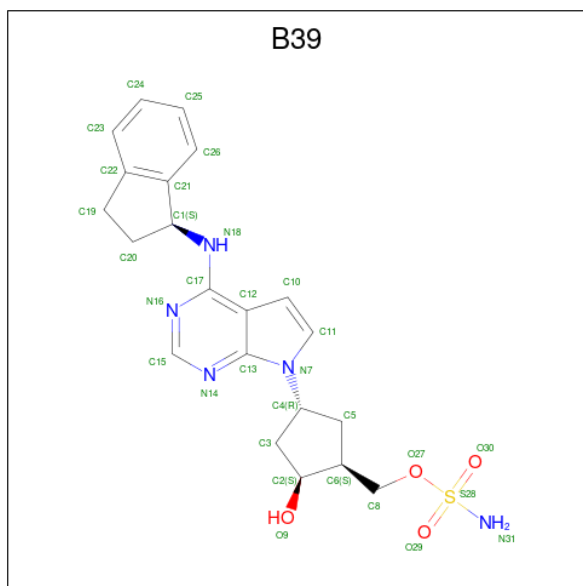
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Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	HIS	-	expression tag	UNP Q15843
J	-2	HIS	-	expression tag	UNP Q15843
J	-1	HIS	-	expression tag	UNP Q15843
J	0	HIS	-	expression tag	UNP Q15843

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

- Molecule 5 is [(1S,2S,4R)-4-{4-[(1S)-2,3-dihydro-1H-inden-1-ylamino]-7H-pyrrolo[2,3-d]pyrimidin-7-yl}-2-hydroxycyclopentyl]methyl sulfamate (CCD ID: B39) (formula: C₂₁H₂₅N₅O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C N O S 31 21 5 4 1	0	0
5	J	1	Total C N O S 31 21 5 4 1	0	0

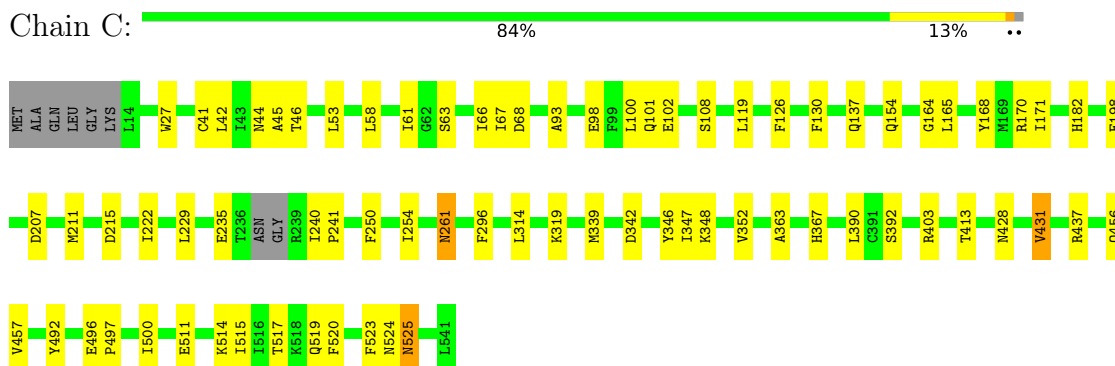
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

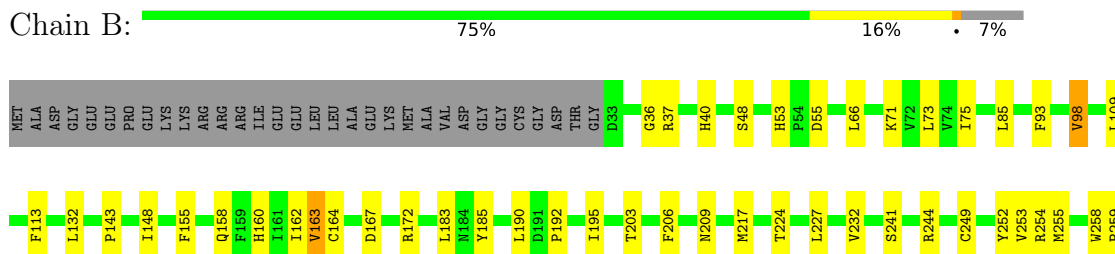
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	135.03Å 228.72Å 229.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 3.00 49.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.36-3.00) 97.3 (49.36-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.287 0.228 , 0.283	Depositor DCC
R_{free} test set	3515 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.428 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16050	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B39, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/4177	0.86	0/5670
1	C	0.53	0/4146	0.86	1/5631 (0.0%)
2	B	0.55	0/3388	0.90	0/4622
2	D	0.55	0/3397	0.92	4/4633 (0.1%)
3	I	0.54	0/600	0.89	1/810 (0.1%)
3	J	0.53	0/609	0.83	0/820
All	All	0.54	0/16317	0.88	6/22186 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	370	LEU	CA-C-N	6.91	128.48	119.84
2	D	370	LEU	C-N-CA	6.91	128.48	119.84
1	C	457	VAL	N-CA-C	5.66	116.30	110.36
2	D	136	VAL	CA-C-N	5.45	125.46	119.90
2	D	136	VAL	C-N-CA	5.45	125.46	119.90
3	I	-1	HIS	N-CA-C	5.15	116.58	111.07

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	A	4095	0	3924	62	0
1	C	4065	0	3883	52	0
2	B	3311	0	3219	53	0
2	D	3320	0	3238	51	0
3	I	593	0	582	6	0
3	J	602	0	598	9	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	I	31	0	23	4	0
5	J	31	0	23	3	0
All	All	16050	0	15490	218	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 (218) 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:D:206:PHE:HB3	2:D:347:ASP:HB3	1.58	0.85
1:C:63:SER:HB3	1:C:108:SER:HB3	1.62	0.81
1:A:182:HIS:HE1	1:A:519:GLN:HE21	1.26	0.81
1:C:182:HIS:CE1	1:C:519:GLN:HE21	2.01	0.79
2:B:75:ILE:HB	2:B:164:CYS:HB3	1.65	0.78
2:B:340:ASN:O	2:B:341:ASN:HB2	1.83	0.76
2:B:185:TYR:CE2	2:B:190:LEU:HB2	2.21	0.74
1:A:314:LEU:HD22	1:A:390:LEU:HD22	1.70	0.74
2:D:204:GLU:HB2	3:J:73:LEU:HD12	1.68	0.74
2:D:209:ASN:ND2	3:J:73:LEU:H	1.85	0.73
1:A:84:GLN:HG3	1:A:99:PHE:CZ	2.22	0.73
1:A:346:TYR:CD2	2:B:244:ARG:HB3	2.24	0.73
1:C:403:ARG:NH2	1:C:413:THR:O	2.21	0.72
1:C:496:GLU:H	2:D:40:HIS:CD2	2.07	0.72
2:B:53:HIS:HD2	2:B:55:ASP:H	1.36	0.71
5:I:464:B39:H1	5:I:464:B39:H10	1.72	0.71
2:B:85:LEU:HB3	2:B:132:LEU:CD1	2.21	0.71
2:B:85:LEU:HB3	2:B:132:LEU:HD11	1.72	0.70
1:C:67:ILE:HD11	1:C:126:PHE:HE2	1.57	0.70
1:A:207:ASP:O	1:A:211:MET:HG3	1.91	0.70
1:A:182:HIS:CE1	1:A:519:GLN:HE21	2.08	0.69
2:B:206:PHE:HB3	2:B:347:ASP:HB3	1.75	0.69
1:C:346:TYR:CD2	2:D:244:ARG:HB3	2.26	0.69
1:A:240:ILE:HB	1:A:241:PRO:CD	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:HIS:HE1	1:C:519:GLN:HE21	1.40	0.69
2:D:340:ASN:O	2:D:341:ASN:HB2	1.93	0.67
1:A:211:MET:HE2	1:A:215:ASP:HB3	1.77	0.66
2:B:167:ASP:HB2	5:I:464:B39:H11	1.76	0.66
1:A:165:LEU:HA	1:A:500:ILE:HG13	1.78	0.66
2:B:71:LYS:H	2:B:160:HIS:HD2	1.45	0.65
2:D:75:ILE:HB	2:D:164:CYS:CB	2.27	0.65
2:D:75:ILE:HB	2:D:164:CYS:HB3	1.80	0.64
2:B:209:ASN:ND2	3:I:73:LEU:H	1.97	0.63
1:A:496:GLU:H	2:B:40:HIS:CD2	2.16	0.62
5:J:464:B39:H10	5:J:464:B39:H1	1.80	0.62
1:A:46:THR:HG21	1:A:137:GLN:HG3	1.82	0.61
2:B:249:CYS:O	2:B:253:VAL:HG23	2.00	0.61
1:C:314:LEU:HD22	1:C:390:LEU:HD22	1.83	0.61
2:B:341:ASN:HB2	2:B:357:GLU:HA	1.82	0.61
1:A:101:GLN:NE2	1:A:109:GLY:H	1.99	0.60
1:C:171:ILE:HD11	1:C:515:ILE:HD11	1.84	0.60
1:A:68:ASP:HB3	1:A:93:ALA:HB2	1.84	0.60
1:C:46:THR:HG21	1:C:137:GLN:HG3	1.83	0.59
3:I:18:GLU:HB2	3:I:21:ASP:OD1	2.03	0.59
1:C:68:ASP:HB3	1:C:93:ALA:HB2	1.85	0.58
2:B:71:LYS:H	2:B:160:HIS:CD2	2.22	0.58
1:A:222:ILE:HD11	1:A:339:MET:HE1	1.86	0.58
1:A:256:GLN:HE21	1:A:256:GLN:HA	1.69	0.58
1:C:496:GLU:H	2:D:40:HIS:HD2	1.51	0.57
1:C:41:CYS:HB2	1:C:130:PHE:CG	2.39	0.57
2:B:386:LEU:HD11	2:B:414:TYR:CD2	2.40	0.57
1:C:46:THR:HG21	1:C:137:GLN:CG	2.35	0.56
1:C:240:ILE:HG13	1:C:241:PRO:HD2	1.86	0.56
2:D:386:LEU:HD11	2:D:414:TYR:CD2	2.41	0.56
1:A:240:ILE:HB	1:A:241:PRO:HD3	1.87	0.56
1:A:372:LEU:HD12	1:A:379:PRO:HA	1.88	0.56
2:D:53:HIS:CD2	2:D:55:ASP:H	2.24	0.56
2:D:53:HIS:HD2	2:D:55:ASP:H	1.55	0.55
1:C:165:LEU:HA	1:C:500:ILE:HG13	1.88	0.55
1:C:207:ASP:O	1:C:211:MET:HG3	2.05	0.55
2:D:406:LEU:HD11	2:D:438:LEU:HD12	1.89	0.55
1:A:46:THR:HG21	1:A:137:GLN:CG	2.37	0.55
2:D:381:LYS:O	2:D:382:LEU:CB	2.55	0.54
2:B:381:LYS:O	2:B:382:LEU:HB2	2.07	0.54
2:B:421:ILE:C	2:B:423:GLU:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:280:TRP:CE2	2:D:284:LYS:HG3	2.43	0.54
2:D:209:ASN:HD21	3:J:73:LEU:H	1.56	0.53
1:A:68:ASP:OD2	1:A:92:ARG:HD2	2.08	0.53
1:C:428:ASN:O	1:C:431:VAL:HG22	2.09	0.53
2:D:341:ASN:HB2	2:D:357:GLU:HA	1.89	0.53
1:C:211:MET:HE2	1:C:215:ASP:HB3	1.90	0.53
1:A:514:LYS:HG2	1:A:520:PHE:HB2	1.90	0.53
2:B:85:LEU:HD21	2:B:98:VAL:HG13	1.91	0.53
1:A:228:TYR:OH	1:A:257:GLY:HA3	2.09	0.53
2:B:307:LYS:HB2	2:B:309:ILE:HG13	1.91	0.53
1:C:27:TRP:HA	1:C:519:GLN:HE22	1.74	0.52
1:C:314:LEU:HB3	1:C:390:LEU:HD22	1.91	0.52
2:D:132:LEU:HD23	2:D:141:VAL:HG21	1.91	0.52
1:A:157:LEU:HD23	1:A:172:ILE:HD12	1.92	0.52
1:A:348:LYS:O	1:A:352:VAL:HG23	2.10	0.51
1:A:71:GLN:HE21	1:A:89:GLY:HA2	1.75	0.51
2:D:386:LEU:HD11	2:D:414:TYR:HD2	1.75	0.51
2:D:330:LYS:HD3	2:D:336:TYR:HB2	1.91	0.51
2:B:53:HIS:CD2	2:B:55:ASP:H	2.24	0.51
2:D:73:LEU:HB3	2:D:162:ILE:HG12	1.92	0.51
1:C:514:LYS:HG2	1:C:520:PHE:HB2	1.92	0.51
1:C:222:ILE:HD11	1:C:339:MET:HE1	1.92	0.50
2:D:162:ILE:HD12	2:D:179:LEU:HD21	1.93	0.50
2:B:381:LYS:O	2:B:382:LEU:CB	2.59	0.50
2:B:71:LYS:N	2:B:160:HIS:HD2	2.08	0.50
2:B:206:PHE:HB3	2:B:347:ASP:CB	2.41	0.50
1:A:67:ILE:HD11	1:A:126:PHE:HE2	1.78	0.49
1:A:381:SER:HB3	2:D:58:PRO:HD2	1.94	0.49
1:A:496:GLU:H	2:B:40:HIS:HD2	1.59	0.49
1:C:42:LEU:HD22	1:C:53:LEU:HD22	1.94	0.49
2:B:386:LEU:HD11	2:B:414:TYR:HD2	1.77	0.49
1:C:53:LEU:HD23	1:C:100:LEU:HD13	1.95	0.49
1:A:491:ARG:HD2	2:B:48:SER:O	2.12	0.49
2:D:224:THR:HB	2:D:227:LEU:HD12	1.94	0.49
2:B:224:THR:HB	2:B:227:LEU:HD12	1.94	0.49
2:D:326:THR:HG22	2:D:330:LYS:HE3	1.94	0.49
1:A:173:ILE:HD11	1:A:515:ILE:HG12	1.94	0.49
1:A:524:ASN:O	1:A:525:ASN:CB	2.60	0.49
2:B:203:THR:HG21	2:B:317:ASN:OD1	2.13	0.49
1:A:58:LEU:HD11	2:B:113:PHE:HB3	1.95	0.48
1:A:256:GLN:HA	1:A:256:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:HD21	2:B:98:VAL:CG1	2.43	0.48
1:C:524:ASN:O	1:C:525:ASN:CB	2.62	0.48
3:I:45:TYR:HB2	3:I:67:LEU:HD22	1.96	0.48
5:I:464:B39:H1	5:I:464:B39:C10	2.37	0.48
1:C:41:CYS:HB2	1:C:130:PHE:CD2	2.49	0.48
2:D:85:LEU:HB3	2:D:132:LEU:HD22	1.96	0.47
1:C:342:ASP:HA	2:D:242:MET:HG2	1.96	0.47
2:D:85:LEU:HD11	2:D:98:VAL:HG11	1.97	0.47
1:A:170:ARG:HA	1:A:525:ASN:O	2.14	0.47
1:A:208:LEU:HD11	1:A:227:LYS:HB3	1.97	0.47
2:B:36:GLY:O	2:B:37:ARG:C	2.58	0.47
2:B:342:TYR:HE2	2:B:344:VAL:HG22	1.78	0.47
1:C:347:ILE:HD11	2:D:294:ILE:HG12	1.97	0.47
2:D:85:LEU:HD21	2:D:98:VAL:CG1	2.45	0.47
1:A:35:LEU:HD11	1:A:513:ILE:HG12	1.97	0.46
2:B:295:ARG:NH1	2:B:295:ARG:HB2	2.30	0.46
1:C:348:LYS:O	1:C:352:VAL:HG23	2.15	0.46
2:B:192:PRO:HA	2:B:195:ILE:HD12	1.97	0.46
1:C:523:PHE:HB3	2:D:351:LEU:HD12	1.98	0.46
2:B:73:LEU:HB3	2:B:162:ILE:HG12	1.98	0.46
5:J:464:B39:H1	5:J:464:B39:C10	2.45	0.46
2:B:66:LEU:HD11	2:B:93:PHE:CE2	2.50	0.46
1:A:41:CYS:HB2	1:A:130:PHE:CD2	2.50	0.46
1:A:195:PRO:HB3	1:A:199:LEU:HD23	1.98	0.46
1:C:164:GLY:HA3	1:C:492:TYR:CG	2.51	0.46
1:C:511:GLU:HG3	1:C:523:PHE:CD2	2.51	0.46
1:A:192:LEU:HD11	1:A:222:ILE:HG23	1.98	0.45
1:C:240:ILE:HG13	1:C:241:PRO:CD	2.46	0.45
1:C:363:ALA:O	1:C:367:HIS:HD2	2.00	0.45
2:B:148:ILE:HD11	5:I:464:B39:H26	1.98	0.45
1:A:41:CYS:HB2	1:A:130:PHE:CG	2.51	0.45
2:B:155:PHE:O	2:B:158:GLN:HG2	2.17	0.45
2:B:183:LEU:HD22	2:B:190:LEU:HD11	1.98	0.45
2:D:148:ILE:HD11	5:J:464:B39:H26	1.97	0.45
2:D:185:TYR:CE2	2:D:190:LEU:HB2	2.51	0.45
1:C:261:ASN:H	1:C:261:ASN:HD22	1.65	0.45
3:J:38:PRO:HA	3:J:41:GLN:HE21	1.82	0.45
1:A:97:MET:HE3	1:A:109:GLY:C	2.41	0.45
2:D:192:PRO:HA	2:D:195:ILE:HD12	1.98	0.45
1:A:511:GLU:HG3	1:A:523:PHE:CD2	2.51	0.45
1:C:250:PHE:CE2	1:C:254:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ARG:NH2	1:A:413:THR:O	2.48	0.45
1:A:517:THR:C	1:A:519:GLN:H	2.25	0.45
2:B:258:TRP:HB3	2:B:259:PRO:HD3	1.97	0.45
2:B:428:ASN:C	2:B:430:SER:H	2.24	0.45
2:D:307:LYS:HB2	2:D:309:ILE:HG13	1.97	0.45
2:D:249:CYS:O	2:D:253:VAL:HG23	2.16	0.45
2:D:85:LEU:HD21	2:D:98:VAL:HG13	1.99	0.44
3:I:35:GLY:O	3:I:37:PRO:HD3	2.17	0.44
2:B:85:LEU:HD11	2:B:98:VAL:HG11	1.99	0.44
2:B:258:TRP:CH2	2:B:277:HIS:CD2	3.05	0.44
1:A:314:LEU:HB3	1:A:390:LEU:HD22	1.99	0.44
1:C:517:THR:C	1:C:519:GLN:H	2.26	0.44
1:A:84:GLN:HG3	1:A:99:PHE:HZ	1.78	0.44
2:B:330:LYS:HG2	2:B:336:TYR:HB2	2.00	0.44
1:C:45:ALA:HB2	1:C:66:ILE:HG21	2.00	0.44
1:A:164:GLY:HA3	1:A:492:TYR:CG	2.53	0.44
1:A:314:LEU:HD21	1:A:382:ILE:HG21	2.00	0.44
1:C:496:GLU:O	1:C:497:PRO:C	2.60	0.44
2:D:183:LEU:HD22	2:D:190:LEU:HD11	2.00	0.43
2:B:252:TYR:C	2:B:252:TYR:CD2	2.96	0.43
2:B:163:VAL:HG21	2:B:328:VAL:HG21	2.01	0.43
1:C:98:GLU:O	1:C:102:GLU:HG3	2.18	0.43
1:A:61:ILE:O	1:A:107:VAL:HG22	2.18	0.43
1:A:42:LEU:HD22	1:A:53:LEU:HD22	2.00	0.43
1:C:198:GLU:N	1:C:198:GLU:OE1	2.52	0.43
2:D:76:GLY:O	2:D:81:GLY:HA3	2.18	0.43
2:D:428:ASN:C	2:D:430:SER:H	2.27	0.43
1:A:308:THR:HG23	1:A:312:TRP:HB2	2.00	0.43
1:A:390:LEU:O	1:A:390:LEU:HG	2.19	0.43
2:D:75:ILE:HB	2:D:164:CYS:HB2	2.00	0.43
3:J:18:GLU:HB2	3:J:21:ASP:OD2	2.18	0.42
3:J:27:LYS:NZ	3:J:52:ASP:OD1	2.48	0.42
1:A:171:ILE:HD11	1:A:515:ILE:HD11	2.01	0.42
1:C:437:ARG:HE	1:C:437:ARG:HB3	1.72	0.42
2:D:53:HIS:HD2	2:D:55:ASP:HB2	1.84	0.42
1:A:42:LEU:CD2	1:A:53:LEU:HD22	2.49	0.42
1:A:45:ALA:HB2	1:A:66:ILE:HG21	2.01	0.42
1:C:296:PHE:HB3	1:C:319:LYS:HE3	2.02	0.42
2:D:160:HIS:C	2:D:161:ILE:HG13	2.45	0.42
2:D:258:TRP:HB3	2:D:259:PRO:HD3	2.01	0.42
1:A:308:THR:HA	1:A:309:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HD11	1:A:126:PHE:CE2	2.55	0.42
1:A:153:SER:O	1:C:456:GLN:NE2	2.52	0.42
1:C:67:ILE:HD11	1:C:126:PHE:CE2	2.45	0.42
3:J:22:LYS:HA	3:J:54:LYS:O	2.19	0.42
1:A:525:ASN:HB3	1:A:539:PHE:O	2.19	0.41
2:B:277:HIS:O	2:B:281:ILE:HD12	2.20	0.41
2:D:85:LEU:HB3	2:D:132:LEU:CD2	2.50	0.41
1:C:46:THR:HG1	1:C:496:GLU:CD	2.28	0.41
2:B:254:ARG:HH21	2:B:255:MET:HE3	1.85	0.41
1:A:168:TYR:CD2	1:A:168:TYR:C	2.98	0.41
2:D:381:LYS:O	2:D:382:LEU:HB2	2.19	0.41
2:B:98:VAL:HG23	2:B:143:PRO:HA	2.03	0.41
1:A:27:TRP:CZ3	1:A:513:ILE:HG21	2.56	0.41
2:B:172:ARG:NH2	3:I:74:ARG:O	2.45	0.41
2:B:319:VAL:O	2:B:323:VAL:HG23	2.21	0.41
1:C:170:ARG:HA	1:C:525:ASN:O	2.20	0.41
1:C:314:LEU:HB3	1:C:390:LEU:CD2	2.51	0.41
1:C:511:GLU:HG3	1:C:523:PHE:HD2	1.86	0.41
2:D:70:CYS:HA	2:D:160:HIS:CD2	2.55	0.41
2:D:426:ARG:N	2:D:427:PRO:HD2	2.35	0.41
3:J:38:PRO:HA	3:J:41:GLN:NE2	2.36	0.41
1:A:314:LEU:HB3	1:A:390:LEU:CD2	2.51	0.40
1:C:497:PRO:HB2	1:C:500:ILE:HG12	2.03	0.40
1:A:170:ARG:HD2	1:A:525:ASN:O	2.22	0.40
2:B:75:ILE:HB	2:B:164:CYS:CB	2.43	0.40
2:D:83:GLU:HG2	2:D:318:ALA:HA	2.03	0.40
3:J:37:PRO:HA	3:J:38:PRO:HD3	1.96	0.40
2:D:380:ALA:O	2:D:381:LYS:CB	2.69	0.40
3:I:26:ILE:O	3:I:30:VAL:HG23	2.21	0.40
1:C:58:LEU:HD11	2:D:113:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	525/534 (98%)	490 (93%)	32 (6%)	3 (1%)	21	56
1	C	522/534 (98%)	493 (94%)	26 (5%)	3 (1%)	21	56
2	B	425/463 (92%)	390 (92%)	30 (7%)	5 (1%)	10	40
2	D	425/463 (92%)	398 (94%)	22 (5%)	5 (1%)	10	40
3	I	77/82 (94%)	71 (92%)	5 (6%)	1 (1%)	9	38
3	J	77/82 (94%)	71 (92%)	5 (6%)	1 (1%)	9	38
All	All	2051/2158 (95%)	1913 (93%)	120 (6%)	18 (1%)	14	48

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	525	ASN
2	B	341	ASN
1	C	525	ASN
2	D	341	ASN
2	D	381	LYS
2	B	241	SER
2	B	382	LEU
2	D	382	LEU
3	J	63	GLY
1	A	327	GLN
1	C	235	GLU
1	A	44	ASN
2	D	371	PRO
2	B	232	VAL
1	C	44	ASN
2	D	231	GLN
2	B	422	GLU
3	I	63	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/464 (94%)	421 (97%)	13 (3%)	36	69
1	C	428/464 (92%)	419 (98%)	9 (2%)	47	75
2	B	357/404 (88%)	345 (97%)	12 (3%)	32	66
2	D	359/404 (89%)	347 (97%)	12 (3%)	33	67
3	I	60/72 (83%)	56 (93%)	4 (7%)	15	46
3	J	61/72 (85%)	57 (93%)	4 (7%)	15	46
All	All	1699/1880 (90%)	1645 (97%)	54 (3%)	34	67

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	119	LEU
1	A	132	VAL
1	A	140	GLU
1	A	178	VAL
1	A	256	GLN
1	A	261	ASN
1	A	270	GLU
1	A	381	SER
1	A	392	SER
1	A	439	VAL
1	A	478	SER
1	A	518	LYS
2	B	98	VAL
2	B	109	LEU
2	B	163	VAL
2	B	217	MET
2	B	287	GLU
2	B	382	LEU
2	B	394	SER
2	B	399	SER
2	B	403	THR
2	B	413	LEU
2	B	444	LEU
2	B	455	VAL
1	C	61	ILE
1	C	101	GLN
1	C	119	LEU
1	C	154	GLN
1	C	168	TYR

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Mol	Chain	Res	Type
1	C	229	LEU
1	C	261	ASN
1	C	392	SER
1	C	431	VAL
2	D	43	LYS
2	D	109	LEU
2	D	207	LYS
2	D	232	VAL
2	D	257	GLN
2	D	281	ILE
2	D	337	ILE
2	D	351	LEU
2	D	369	GLN
2	D	406	LEU
2	D	413	LEU
2	D	455	VAL
3	I	2	LEU
3	I	17	ILE
3	I	70	VAL
3	I	71	LEU
3	J	2	LEU
3	J	17	ILE
3	J	70	VAL
3	J	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	152	ASN
1	A	182	HIS
1	A	202	HIS
1	A	218	HIS
1	A	256	GLN
1	A	307	GLN
1	A	329	ASN
1	A	366	ASN
1	A	443	HIS
1	A	456	GLN
1	A	487	HIS
1	A	519	GLN
1	A	525	ASN

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Mol	Chain	Res	Type
2	B	40	HIS
2	B	53	HIS
2	B	138	ASN
2	B	152	ASN
2	B	160	HIS
2	B	209	ASN
2	B	277	HIS
2	B	341	ASN
2	B	363	ASN
1	C	71	GLN
1	C	101	GLN
1	C	152	ASN
1	C	176	HIS
1	C	182	HIS
1	C	256	GLN
1	C	261	ASN
1	C	329	ASN
1	C	366	ASN
1	C	443	HIS
1	C	456	GLN
1	C	510	GLN
1	C	519	GLN
2	D	40	HIS
2	D	53	HIS
2	D	158	GLN
2	D	160	HIS
2	D	209	ASN
2	D	277	HIS
2	D	340	ASN
2	D	341	ASN
2	D	410	ASN
3	I	-1	HIS
3	I	41	GLN
3	J	49	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	B39	I	464	3	35,35,35	2.88	7 (20%)	40,52,52	2.91	12 (30%)
5	B39	J	464	3	35,35,35	2.95	7 (20%)	40,52,52	2.85	13 (32%)

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
5	B39	I	464	3	-	3/14/35/35	0/5/5/5
5	B39	J	464	3	-	2/14/35/35	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	464	B39	O27-S28	-10.76	1.43	1.57
5	I	464	B39	O27-S28	-9.99	1.44	1.57
5	I	464	B39	O30-S28	7.22	1.50	1.42
5	I	464	B39	O29-S28	7.16	1.50	1.42
5	J	464	B39	O30-S28	7.06	1.49	1.42
5	J	464	B39	O29-S28	6.90	1.49	1.42
5	J	464	B39	S28-N31	5.10	1.64	1.58
5	J	464	B39	C11-N7	-4.93	1.33	1.39
5	I	464	B39	C11-N7	-4.92	1.33	1.39
5	I	464	B39	S28-N31	4.90	1.64	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	464	B39	C12-C10	-3.12	1.33	1.44
5	I	464	B39	C12-C10	-3.07	1.34	1.44
5	I	464	B39	C1-N18	2.16	1.48	1.45
5	J	464	B39	C1-N18	2.08	1.48	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	464	B39	O30-S28-O29	-11.87	107.86	119.94
5	I	464	B39	O30-S28-O29	-11.39	108.35	119.94
5	I	464	B39	C8-O27-S28	7.15	126.43	117.29
5	J	464	B39	C8-O27-S28	5.54	124.37	117.29
5	I	464	B39	C12-C13-N14	-4.79	118.44	126.89
5	I	464	B39	N14-C15-N16	-4.77	121.37	128.58
5	J	464	B39	N14-C15-N16	-4.76	121.37	128.58
5	J	464	B39	C12-C13-N14	-4.52	118.93	126.89
5	I	464	B39	N14-C13-N7	4.41	134.67	127.17
5	J	464	B39	N14-C13-N7	4.03	134.02	127.17
5	I	464	B39	C15-N14-C13	4.00	121.60	111.83
5	J	464	B39	C15-N14-C13	3.79	121.10	111.83
5	J	464	B39	C10-C11-N7	-3.53	107.56	110.31
5	I	464	B39	C12-C13-N7	-3.26	106.89	108.28
5	J	464	B39	C13-N7-C11	3.20	109.43	107.95
5	J	464	B39	C12-C10-C11	3.13	109.70	107.01
5	I	464	B39	C10-C11-N7	-3.02	107.96	110.31
5	I	464	B39	C12-C10-C11	2.98	109.57	107.01
5	J	464	B39	C12-C13-N7	-2.87	107.05	108.28
5	I	464	B39	C13-N7-C11	2.59	109.15	107.95
5	J	464	B39	C19-C20-C1	-2.59	101.57	105.59
5	I	464	B39	C19-C20-C1	-2.35	101.95	105.59
5	J	464	B39	C19-C22-C21	-2.06	108.58	110.69
5	I	464	B39	O27-S28-N31	2.06	112.17	105.54
5	J	464	B39	O27-S28-N31	2.03	112.08	105.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	464	B39	C12-C17-N18-C1
5	J	464	B39	C12-C17-N18-C1
5	I	464	B39	N16-C17-N18-C1
5	J	464	B39	N16-C17-N18-C1

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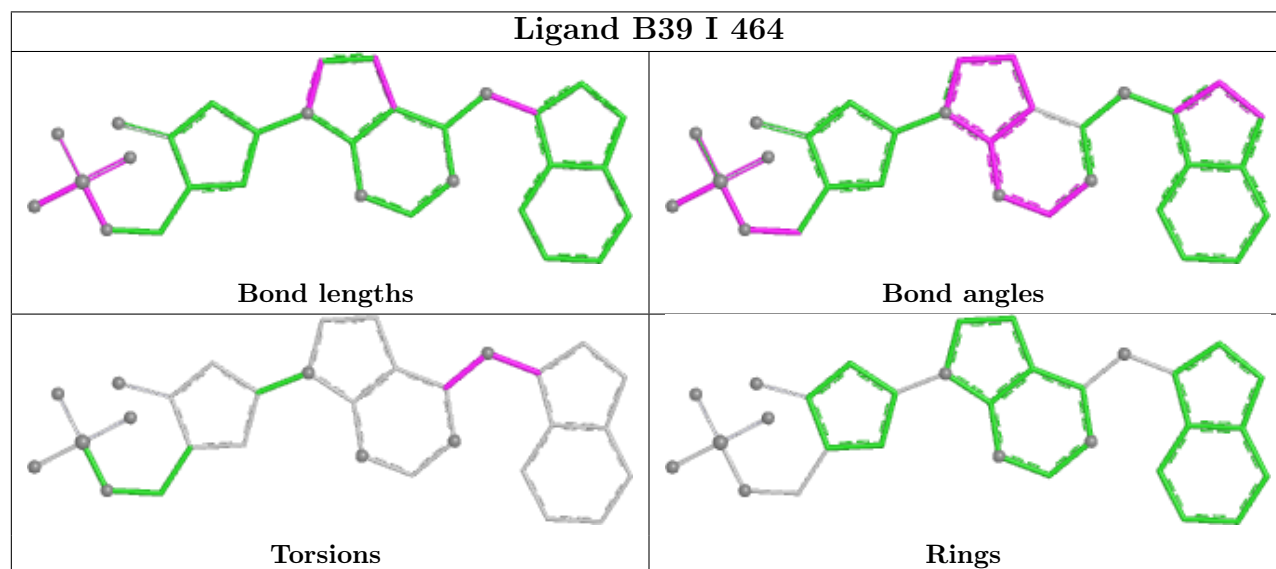
Mol	Chain	Res	Type	Atoms
5	I	464	B39	C20-C1-N18-C17

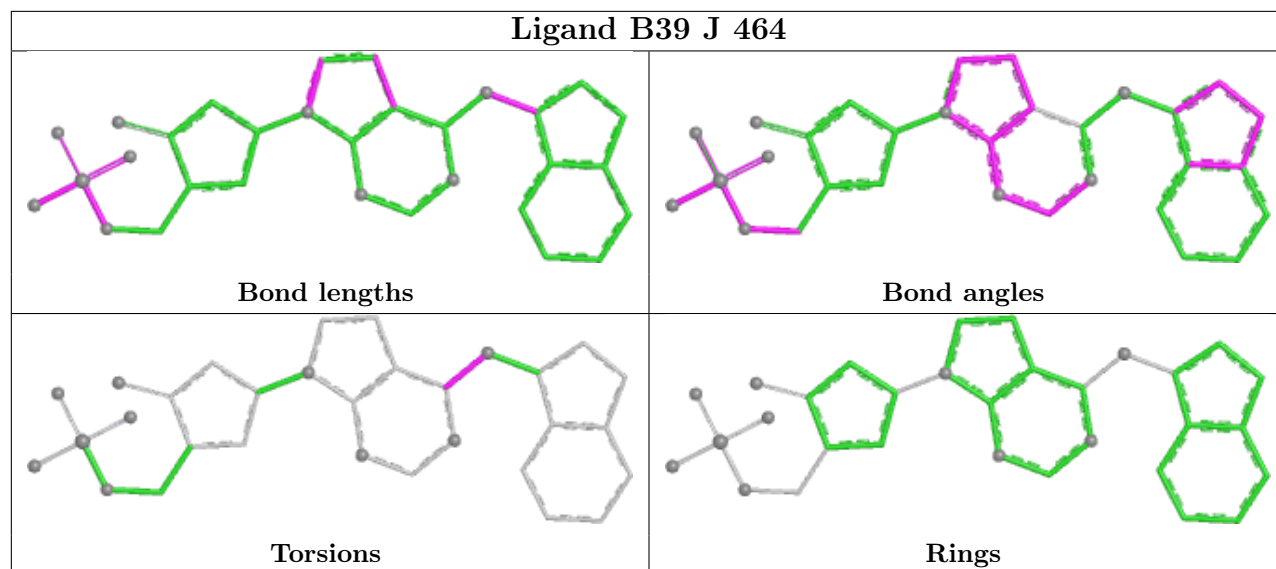
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	464	B39	4	0
5	J	464	B39	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	527/534 (98%)	-1.00	0 100 100	42, 63, 104, 109	0
1	C	526/534 (98%)	-1.00	0 100 100	44, 63, 102, 112	0
2	B	429/463 (92%)	-1.04	0 100 100	45, 64, 100, 116	0
2	D	429/463 (92%)	-1.01	0 100 100	46, 63, 100, 118	0
3	I	79/82 (96%)	-1.16	0 100 100	47, 65, 75, 79	0
3	J	79/82 (96%)	-1.16	0 100 100	48, 65, 75, 82	0
All	All	2069/2158 (95%)	-1.02	0 100 100	42, 64, 102, 118	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	B39	I	464	31/31	0.99	0.04	48,56,60,60	4

Continued on next page...

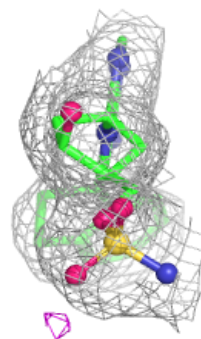
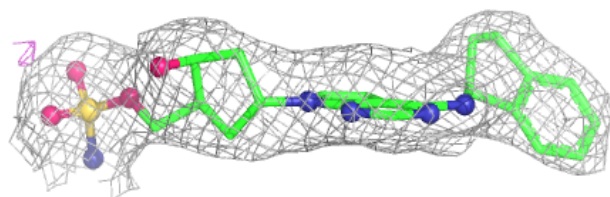
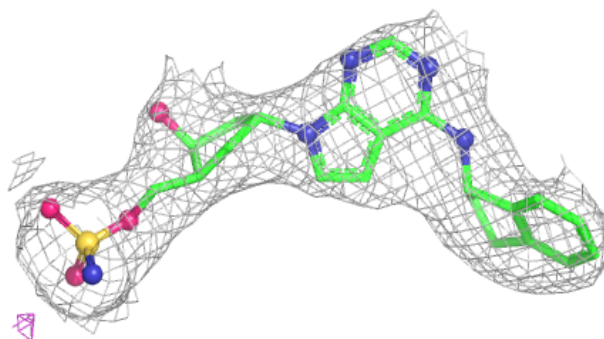
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	B39	J	464	31/31	0.99	0.04	50,55,60,60	4
4	ZN	B	465	1/1	1.00	0.01	56,56,56,56	0
4	ZN	D	465	1/1	1.00	0.01	56,56,56,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

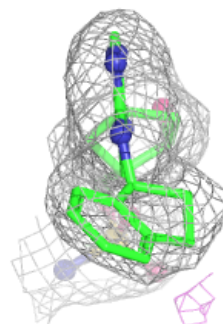
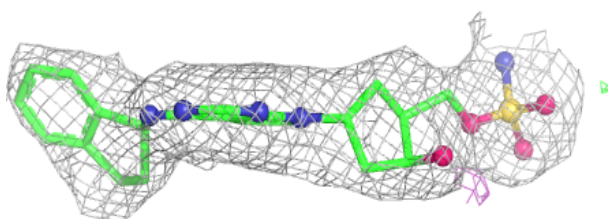
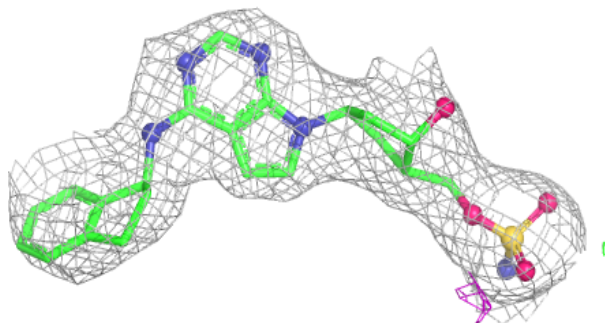
Electron density around B39 I 464:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B39 J 464:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.